Report

Model Development and Remedial Wellfield Optimization Report

Dual Site Groundwater Operable Unit Remedial Design Montrose Chemical and Del Amo Superfund Sites

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3 Hutton Centre Drive, Suite 200 Santa Ana, California 92707

MODEL DEVELOPMENT AND REMEDIAL WELLFIELD OPTIMIZATION REPORT DUAL SITE GROUNDWATER OPERABLE UNIT REMEDIAL DESIGN MONTROSE CHEMICAL AND DEL AMO SUPERFUND SITES

United States Environmental Protection Agency Region 9 75 Hawthorne Street San Francisco, California 94105 CH2M HILL Project No. 335380.PD.03

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Acronyms and Abbreviations

AST aboveground storage tank

CZ containment zone

DDT dichlorodiphenyltrichloroethane

D_L longitudinal dispersivity

DNAPL dense nonaqueous phase liquid

D_T transverse to longitudinal dispersivity

DTSC Department of Toxic Substances Control

Dual Site Montrose Chemical and Del Amo Superfund Dual Site

D_Z vertical to longitudinal dispersivity

EPA United States Environmental Protection Agency

ft/day feet per day

ft/ft

FS feasibility study

FTP file transfer protocol (site on the Internet)

g/cm³ grams per cubic centimeter

foot per foot

GHB general-head boundary

GLA Gage-Lynwood aquitard

gpm gallons per minute

H+A Hargis + Associates

HSU hydrostratigraphic unit

in./yr inches per year

ISGS in situ groundwater standards

JGWFS Joint Groundwater Feasibility Study

K hydraulic conductivity

Kd distribution coefficient

kg/m³ kilograms per cubic meter

Kh horizontal hydraulic conductivity

Kv vertical hydraulic conductivity

LBF Lower Bellflower aquitard

LNAPL light nonaqueous phase liquid

μg/L micrograms per liter

MACP Monitoring and Compliance Plan

MBFB Middle Bellflower B-Sand

MBFC Middle Bellflower C-Sand

MBFM Middle Bellflower Mud

MCL maximum contaminant level

ml/g milliliters per gram

Montrose Chemical Corporation of California

NAD North American Datum

NAPL nonaqueous phase liquid

OOD Overall Operational Design

p-CBSA parachlorobenzene sulfonic acid

R retardation factor

RD remedial design

RI remedial investigation

RMS root mean squared

ROD Record of Decision

Shell Oil Company

TCE trichloroethene

TI technical impracticability

UBA Upper Bellflower aquitard (Montrose nomenclature)

UBF Upper Bellflower aquitard (Del Amo nomenclature)

USGS United States Geological Survey

VOC volatile organic compound

1. Introduction

This report discusses the development and calibration of the remedial design (RD) model and optimization of the remedial wellfield for the Dual Site Groundwater Operable Unit RD for the Montrose Chemical and Del Amo Superfund Sites (Dual Site), located in Los Angeles County California (Figure 1-1). The results of the modeling activities discussed in this report were used to develop the Overall Operational Design (OOD), which includes a set of design specifications for the initial remedial wellfield. The OOD is presented in a separate report (CH2M HILL, 2008).

1.1 Objectives of Model Development and Remedial Wellfield Optimization

The Record of Decision (ROD) for the Dual Site Groundwater Operable Unit issued by the United States Environmental Protection Agency (EPA) on March 30, 1999 (ROD) selected a remedy for the dissolved-phase contamination at the site, and mandated that the RD model be used for the development and optimization of the remedial wellfield. The ROD also required that the remedial wellfield meet a number of design requirements and objectives. The detailed requirements of the ROD appear primarily in ROD Section 13 (EPA, 1999). Some of the most critical ROD requirements pertaining to the development of the remedial wellfield include the following:

- A total pumping rate for the remedial wellfield that is not less than 700 gallons per minute (gpm);
- Indefinite containment of all contaminants presently within a zone that the ROD refers to as the containment zone (CZ);
- Containment of the overall distribution of Dual Site contaminants;
- Reduction of the volume of water with concentrations of contaminants above drinking water standards to zero, progress toward which is required within certain timeframes;
- Achieving certain pore-volume flushing rates within the contaminant distributions;
- The limiting of adverse migration of significant contaminants, either as concentrations in the dissolved phase, or nonaqueous phase liquid (NAPL), especially to hydrostratigraphic layers lying below the present contamination; to this end, wells and pumping are required to reverse or otherwise control downward gradients; and

• The redistribution of groundwater extraction as the contaminant plume shrinks,¹ from clean areas to remaining contaminated areas, to expedite overall cleanup and make it more efficient.

The primary general objective of the modeling activities was to meet the requirements of the ROD with regard to the development and optimization of the remedial wellfield. The specific objectives included the following:

- Development and calibration of the numerical RD model, which is accepted by EPA, Shell Oil Company (Shell), Montrose Chemical Corporation of California (Montrose), and other stakeholders as an appropriate tool for the optimization of the remedial wellfield;
- Development and optimization of the remedial wellfield;
- Failure analysis of the remedial wellfield to ensure that it can meet ROD requirements with a sufficient degree of certainty, and in a manner sufficiently robust to succeed even if actual site conditions differ from those assumed or change in the future; and
- Development of the OOD that meets all ROD requirements.

1.2 Project Background and Overview

The original numerical model of the Dual Site was developed as part of the Joint Groundwater Feasibility Study (JGWFS) to compare remedial alternatives. The JGWFS model was developed by Montrose, and by Shell Chemical Company (Shell), who are the potentially responsible parties and are conducting the remedial design under EPA order. The JGWFS model is discussed in detail in the Final JGWFS for the Montrose and Del Amo Sites, Appendix B (CH2M HILL, 1998). The JGWFS model was revised as part of the initial calibration and data gap analysis, which were performed during RD to quantify the predictive uncertainty of the model, and to identify data types that could have the greatest effect in reducing this uncertainty (i.e., identify data gaps). The results of this analysis are discussed in detail in the Initial Calibration and Data Gap Analysis Report (CH2M HILL, 2005). Extensive additional data acquisition activities were performed by Montrose and Shell during RD to address the data gaps identified by modeling and also to provide additional data required by the ROD.

The RD model described in this report was constructed and calibrated based on the most complete and comprehensive data set available at this time, including data collected during the remedial investigation/feasibility study (RI/FS) and RD phases by Shell, Montrose, and other parties. These data include hydrostratigraphic information from numerous soil borings, contaminant concentration and water level measurements collected over a period of 1985 through 2006, and the results of extensive pilot-scale extraction and injection testing.

¹ Redistribution means shutting down a well(s) on the downgradient end of a shrinking plume once the well is in clean groundwater. Further, the pumping rate would be increased in other active well(s) upgradient within the remaining plume by an amount required to expedite overall cleanup, make cleanup more efficient, and meet the requirements of the ROD. The same effect could be achieved by distributing the pumping to a newly installed well(s).

Model calibration and optimization of the remedial wellfield were performed using the parameter estimation software package PEST (Doherty, 2002; Doherty and Johnston, 2003), which allowed automatic calibration (versus traditional manual calibration, which is a more time-consuming and less-effective process). In addition, the use of PEST allowed cost-effective optimization of the remedial wellfield and failure analysis to ensure that the wellfield can perform reasonably well under a range of plausible conditions.

All modeling activities (including model development, model calibration, and remedial wellfield optimization and failure analysis) were conducted with the oversight and regular involvement of Montrose and Shell. All modeling files were provided at the CH2M HILL file transfer protocol (FTP) site on the Internet for review on a regular basis. The results of this review were discussed at modeling meetings and/or regular modeling conference calls, so that input from Shell, Montrose, EPA, and the Department of Toxic Substances Control (DTSC) could be incorporated in a timely manner at every step of the modeling process. All final numerical model files for the model calibration and optimization of the remedial wellfield were also provided at the CH2M HILL FTP site.

1.3 Report Organization

The report consists of the following sections; figures are provided at the end of each section:

- Section 1, Introduction Discusses the objectives of the modeling activities, project background and overview, the organization of his report, and the definition of terms used in this report.
- **Section 2, Model Development** Discusses the conceptual and numerical model of the Dual Site.
- **Section 3, Model Calibration** Discusses calibration methodology and calibration results.
- **Section 4, Wellfield Optimization** Discusses the optimization methodology and the results of the remedial wellfield optimization.
- **Section 5, Wellfield Failure Analysis** Discusses the methodology and results of the remedial wellfield failure analysis.
- **Section 6, Conclusions and Recommendations** Presents conclusion and recommendations based on the findings of these modeling activities.
- Section 7, References Presents a list of bibliographic references used in this report.

The following appendixes also are included in this report:

- Appendix A Electronic Copy of Baseline Calibrated Model and Optimized Wellfield Simulation
- **Appendix B** Electronic Copy of Simulated Pilot Test Hydrographs
- Appendix C Modifications to MT3DMS Code

- Appendix D—Electronic Copy of Simulated Chlorobenzene, Benzene, and p-CBSA Chemographs
- **Appendix E**-3D Animations of Optimized Wellfield Performance

1.4 Definitions of Terms

This section contains definitions of several important terms used repeatedly in this document. The terms used in this report are consistent with those used in the ROD. The ROD provides requirements, some of which differ by areas defined in the ROD such as the chlorobenzene plume, benzene plume, trichloroethene (TCE) plume, and containment zone (CZ). This document assumes a familiarity with these concepts, which are defined in detail in the ROD.

Wellfield configuration – The spatial layout (locations) of extraction and injection wells for each hydrostratigraphic unit (HSU) from which extraction and injection are required.

Remedial wellfield – Wellfield configuration combined with a pumping schedule (for example, location, HSU, and specified extraction rates through time for each well).

Calibration target - A field measurement (for example, a water level or contaminant concentration measured at a specific well at a specific time), or an estimate derived from field measurements (for example, a water-level difference computed from two water-level measurements). The calibration process attempts to adjust model properties so that simulated values match these measurements.

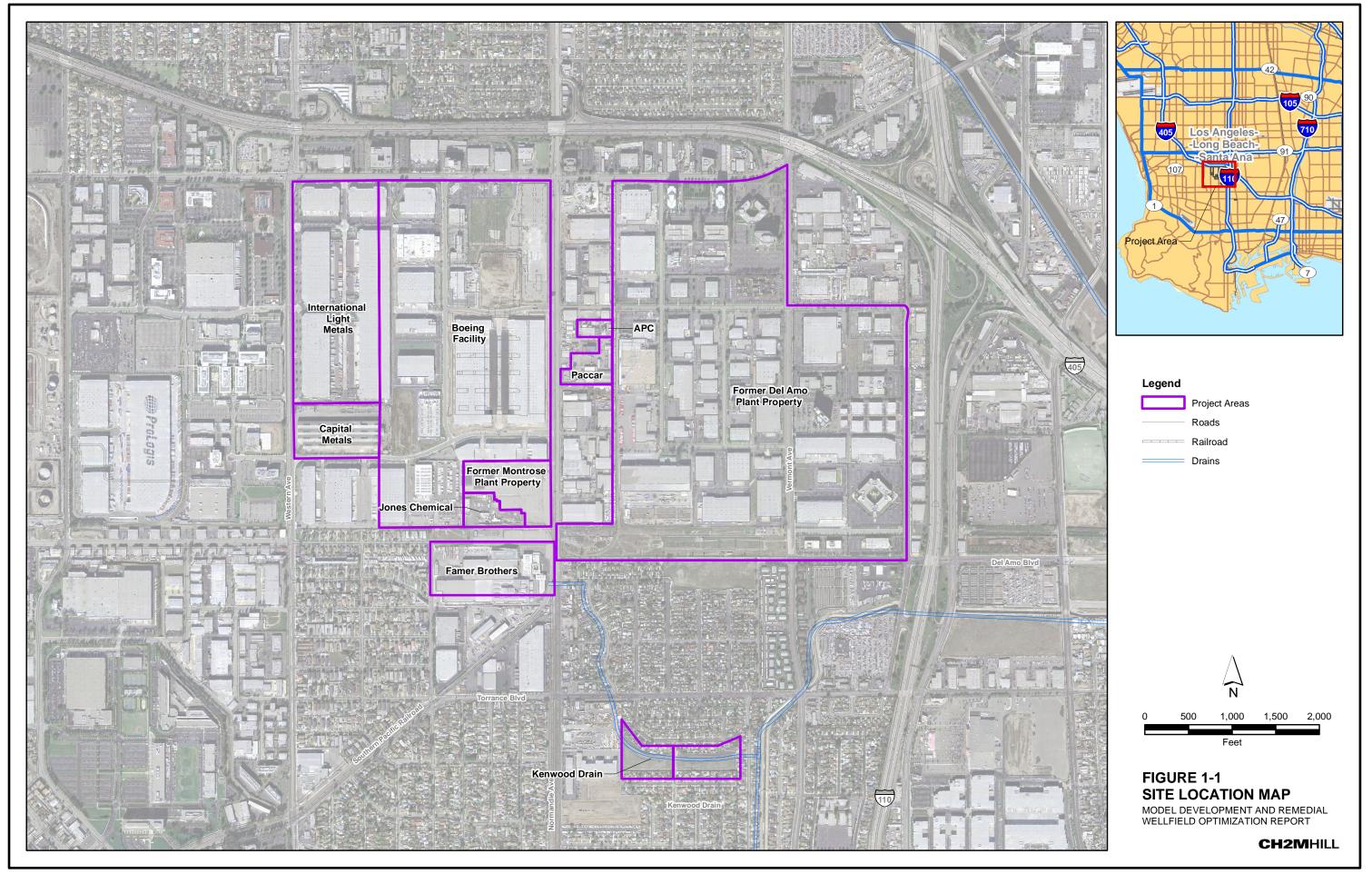
Remediation target – A numerical representation derived from the ROD remedial objectives and standards incorporated as targets into optimization simulations (for example, pump rate, plume containment, plume volume reduction, etc.).

Design constraint – An enforced limit on the RD (for example, feasible locations for wells and well-specific production capacities).

Optimization target – A numerical representation of a design characteristic that is preferred, but not required.

CZ containment well – An extraction or injection well that has, as a primary purpose, the maintenance of containment of dissolved-phase contaminants within the CZ, including the limiting of vertical adverse migration from shallower to deeper HSUs (for example, reversing downward hydraulic gradients through extraction or injection).

Plume-reduction well – An extraction well that has, as a primary purpose, the reduction of the volume of the chlorobenzene plume outside the CZ, within the target timeframes specified in the ROD.



Model Development

This section discusses the conceptual and numerical model of the Dual Site including code selection, model geometry, boundary conditions and recharge, model layers, hydraulic and transport properties, and water levels. It also discusses distribution of contaminant plumes including chlorobenzene, benzene, parachlorobenzene sulfonic acid (p-CBSA), and TCE used for model calibration and optimization of the remedial wellfield.

2.1 Code Selection

The groundwater flow model MODFLOW-2000 (United States Geological Survey [USGS], 2000), the solute-transport model MT3DMS (Zheng and Wang, 1999), and the particle-tracking code MODPATH (USGS, 1994) were used for the development of the RD model. MODFLOW-2000 and MT3DMS are the updated versions of the numerical flow and transport codes that were used for the JGWFS model (i.e., MODFLOW [USGS, 1988] and MT3D96 [S.S. Papadopulos & Associates, 1996]). These codes are widely accepted by the regulatory community, and are used extensively by EPA at numerous sites across the country, primarily because these codes are in the public domain, are well-documented, and have been verified against a number of analytical solutions.

Model calibration and optimization of the remedial wellfield were performed using the parameter estimation software package PEST (Doherty, 2002; Doherty and Johnston, 2003). The use of PEST allowed:

- 1. Automatic model calibration (versus traditional manual calibration, which is a more time-consuming and less-effective process);
- 2. Calibration to multiple target types (e.g., hydraulic heads, vertical head differences, pilot test data, and concentrations of chlorobenzene, benzene, and p-CBSA);
- 3. Numerical uncertainty and data gap analysis, which allowed identification of additional contamination in the Gage aquifer;
- 4. Development and optimization of the remedial wellfield, which is capable of achieving all remedial objectives of the ROD in a cost-effective manner and with a reasonable degree of certainty; and finally
- 5. Failure analysis of the remedial wellfield in order to assess the impact of modeling uncertainties on the wellfield performance.

2.2 Model Geometry

The model domain is a rectangular area roughly centered on the Dual Site and extending laterally beyond the site boundary (see Figure 2-1). As discussed in the ROD, the Dual Site consists of:

- 1. The former Montrose and Del Amo properties
- 2. The areas of groundwater contamination originating from these properties
- 3. The areas of groundwater contamination originating from other adjacent sources that partially or completely overlap with contamination originating from the former Montrose and Del Amo properties and could be impacted by the selected remedial actions.

The model domain extends over an area of approximately 5,400 acres or 8.5 square miles. It is oriented in a northwest to southeast direction, approximately parallel to the predominant groundwater flow direction in the principal HSUs.

The model grid consists of 166 rows, 126 columns, and 13 layers, for a total of 271,908 cells, 264,620 of which are active in simulations. Most model cells are 100 feet by 100 feet square, with 16 columns of 200-foot by 100-foot cells along the northern edge. The model grid was refined by a factor of two from its original size (mostly 200-foot by 200-foot cells) to reduce numerical dispersion during solute transport simulations of the benzene and chlorobenzene plumes. As discussed in Interim Modeling Memorandum No. 16: Grid Refinement Issues and Responses to Shell's April 19, 2006 Letter (CH2M HILL, 2006b), this grid size was selected by running the model with several refined grids and identifying a grid spacing that could be used without significantly compromising the accuracy of results. This grid size was selected to balance the increase in run time caused by smaller grid spacing with the benefit of more accurate modeling predictions due to decreased numerical dispersion.

Vertically, the model is divided into 13 layers of variable thickness that represent 8 HSUs identified to depths of approximately 400 feet beneath the Dual Site (see Table 2-1). Model layers were defined using numerous site-specific hydrostratigraphic data collected during the RI and RD investigations, including additional Gage aquifer investigations performed based on the results of the data gap analysis to assess the extent of the chlorobenzene plume. The locations of lithologic control data within the model domain are shown in Figure 2-2, and a summary of the hydrostratigraphic control data is presented in Table 2-2.

To ensure sufficient numerical accuracy in model simulations, the Lower Bellflower aquitard (LBF) and Gage-Lynwood aquitard (GLA) were subdivided into three model layers each; and the Middle Bellflower C-Sand (MBFC) was subdivided into two model layers, MBFCl and MBFC2 (layers 4 and 5, respectively). Because of the limited data for the Lynwood aquifer, the bottom model layer (layer 13) representing the Lynwood aquifer was assigned a thickness of 50 feet, which is approximately half of the known thickness of the Lynwood aquifer. This layer serves as a vertical (bottom) boundary of the model. Figures 2-3A through 2-3H show interpreted elevation contours of the base of each HSU.

TABLE 2-1 Hydrostratigraphic Units and Model Layers

	Hydrostratigraphic	Units (HSUs)	
Del Amo Nomenci	ature and HSU No.	Montrose Nomenclature	Model Layers
Upper Bellflower Aqu	itard (UBF) – 1	Upper Bellflower Aquitard (UBA)	1
Middle Bellflower	MBFB – 2		2
Aquitard (MBF)	MBFM - 3		3
	MBFC – 4	Bellflower Sand	4 and 5
Lower Bellflower Aqu	itard (LBF) – 5	Lower Bellflower Aquitard (LBF)	6, 7, 8
Gage Aquifer – 6		Gage Aquifer	9
Gage-Lynwood Aquit	ard (GLA) – 7	Gage-Lynwood Aquitard (GLA)	10, 11, 12
Lynwood Aquifer – 8		Lynwood Aquifer	13

2.3 Boundary Conditions

A combination of general-head and no-flow boundaries was used for the numerical model of the Dual Site. General-head boundaries (GHBs) were used to allow hydraulic head to vary under different hydraulic stresses during simulations of remedial pumping and injection. For each GHB cell, a reference head was assigned outside the model domain, and corresponding values of conductance were derived to reproduce the interpreted water levels at the model boundaries. GHBs in the aquitards were estimated from measured water-level elevations in the overlying and underlying aquifers, and were based on the assumption of steady flow conditions (see Section 2.4). Specifically, four to seven points were defined along the model boundaries based on the 2006 baseline water-level contours extrapolated to the edges of the model domain. The number and locations of these points depended on the availability of water-level data in the vicinity of the model boundaries in each HSU. GHBs between these points were derived by interpolation of water levels between these points.

In addition, a small number of no-flow or zero-flux cells were used in certain boundary segments of the Upper Bellflower aquitard (UBF) and the Middle Bellflower Mud (MBFM) where these units are unsaturated (Section 2 of the JGWFS, CH2M HILL, 1998). The Dominguez Channel was simulated using the river package in MODFLOW (USGS, 1988). Model boundary conditions are shown in Figure 2-1.

In the transport model, the GHBs were treated as source/sink terms with the concentration at the reference location prescribed at zero. Cells with constant concentrations were used to simulate the NAPL sources and other areas with persisting detected contaminant concentrations in groundwater. The source concentrations were estimated from 2006 baseline concentration data. The development of the source terms is discussed further in Section 2.8 of this report.

Boundary conditions were adjusted to match measured water-level elevations and contaminant concentrations during the calibration process. To the extent possible, the boundaries were set at sufficient distances away from areas proposed for pumping and injection in order to minimize the impacts on groundwater flow and migration of dissolved contaminants. Water-level drawdowns and other effects of the flow and transport simulations were determined to be insignificant at the model boundaries.

2.4 Groundwater Flow Conditions

The 2006 baseline water level data were used for the calibration of the numerical model (see Figure 2-4). Steady-state conditions were assumed to be appropriate for these simulations because of the following facts:

- The West Coast Basin is overlain by the low-permeability fine-grained Bellflower aquitard, and seasonal changes in the amount of recharge do not significantly affect groundwater levels.
- The total regional groundwater production from the West Coast Basin is essentially constant because the basin is adjudicated.
- A rising trend in the groundwater elevations appears to be uniform and similar in all of
 the units of interest (units within the Bellflower aquitard and the Gage and Lynwood
 aquifers); and therefore, horizontal and vertical components of hydraulic gradient in
 these units do not change significantly in response to this rise (see Section 2 of the
 JGWFS, CH2M HILL, 1998).

Based on the above, the impact of this rise of water levels on the model simulations is not expected to be significant. It also is anticipated that water levels at the Dual Site would approach steady-state shortly after the start of the remedial actions (i.e., drawdown and mounding in the remedial extraction and injection wells, respectively, will stabilize in a short period of time relative to an overall remedy implementation). This was confirmed by the pilot extraction and injection testing, which indicated that water levels stabilize relatively quickly during pilot pumping and or injection. This comprehensive pilot program was implemented by Montrose to obtain data on the hydraulic properties of the aquifers and aquitards, and specific capacities of injection and extraction wells. The pilot testing program included six extraction and four injection tests of relatively long duration (up to 5 days) and with relatively high flow rates (up to several hundred gpm). In addition, three additional 12-hour aquifer tests were performed using monitoring wells at the downgradient edge of the chlorobenzene plume in the MBFC. A detailed discussion of the pilot testing program is included in the Pilot Extraction and Aquifer Response Test Completion Report (Hargis + Associates [H+A], 2008).

TABLE 2-2

Hydrostratigraphic Control Points

							_	Bas	se Elevatio	n ¹ of Hydro	stratigrap	hic Unit	_			
Location	X-coordinates ²	Y-coordinates ²	Reference Elevation ¹	UBF	MBFB	MBFM	MBFC1	MBFC2	LBF1	LBF2	LBF3	Gage	GLA1	GLA2	GLA3	Lynwood
BL-10B&C	4195754	4058949	56		-39	-53	-58.00	-63	-70.00	-77.00	-84	> -99				
BL-11B&C	4195771	4057839	56		-44	-53	-58.00	-63	-70.00	-77.00	-84	> -99				
BL-12C	4195487	4058083	56.25		-26.25	-41.75	-65.25	-78.25	-80.75	-83.25	-85.75					
BL-13C	4196049	4057119	53.41		-37.09	-41.59	-58.84	-76.09	-82.09	-88.09	-94.09					
BL-9B	4195784	4059830	53		-42	-55		> -66								
Carson 2	4202704	4047843	40								-90	-155	-158.33	-161.67	-165	-215
CPL0005	4198505	4057792	37.47	-33												
CPL0009	4199559	4057676	32.8	-44												
CPL0011	4197437	4056540	42.45	-16	-38	-41										
CPT-1	4199266	4056201	33.45	-34												
CPT-11	4199532	4056718	34.2	-42												
CPT-12	4199448	4056533	34	-38												
CPT-13	4199181	4056520	34.47	-34												
CPT-14	4199030	4056521	35.04	-34												
CPT-15	4198879	4056516	35.5	-34												
CPT-16	4198729	4056518	35.83	-33												
CPT-17	4199084	4056721	36.27	-36												
CPT-18	4198939	4056720	36.84	-33												
CPT-2	4198211	4056172	37.99	-17												
CPT-3	4199594	4056220	27.28	-42												
CPT-4	4198847	4056449	32.19	-33												
CPT-5	4199712	4056474	30.4	-41												
CPT-6	4199910	4056420	29.8	-46												
CPT-7	4199333	4056521	33.52	-37												
CPT-8	4199532	4056510	32.6	-40												
DB-1	4194319	4058333	54.7		-46.3	-50.3	-59.80	-69.3	-72.63	-75.97	-79.3	-165.3				
DB-2	4195364	4060761	49.7		-51.3	-55.3	-60.80	-66.3	-77.3	-86.3	-91.3	-168.3				
EB-18	4202113	4052362	34.93					-113.57	-115.07	-116.57	-118.07	>-167.07				
EB-19	4198942	4054829	37.93					-101.37	-107.37	-113.37	-119.37	-166.07				
EB-20	4195863	4055486	46.48					-67.52	-69.02	-70.52	-72.02	>-152.02				
EB-21	4196831	4053430	35.96					-84.04	-85.71	-87.37	-89.04	>-164.04	-170.00	-175.00	-180	
EB-22	4198327	4052776	24.95					-87.25	-88.85	-90.45	-92.05	-156.05				
EB-23	4198680	4054176	31.4					-93.9	-98.80	-103.70	-108.6	-164.9				
EB-25	4199886	4056660	34.5					-107.5	-115.50	-123.50	-131.5	-186.5				
EB-26	4194654	4057065	55.41		-43	-52	-60.80	-69.59	-72.92	-76.26	-79.59	-157				
EB-27	4197434	4056542	42.1					-71.9	-81.03	-90.17	-99.3					
EB-28	4194924	4055578	50.42					-74.58	-78.58	-82.58	-86.58	>-149.58				
EB-29	4195114	4053641	45.38					-74.62	-77.55	-80.49	-83.42	-156.02				
EB-30	4200748	4051398	36.56		†			-78.44	-85.31	-92.17	-99.04	-156.34				

TABLE 2-2
Hydrostratigraphic Control Points

								Bas	se Elevation	n ¹ of Hydro	stratigrap	hic Unit				
Location	X-coordinates ²	Y-coordinates ²	Reference Elevation ¹	UBF	MBFB	MBFM	MBFC1	MBFC2	LBF1	LBF2	LBF3	Gage	GLA1	GLA2	GLA3	Lynwood
EB-31	4202580	4050665	36.92					-68.08	-78.91	-89.75	-100.58	-162.58				
EB-32	4201359	4053430	32.68					-115.62	-122.42	-129.22	-136.02	>-167.32				
EB-33	4202922	4052014	32.93					-110.57	-114.64	-118.70	-122.77	>-168.07				
EB-34	4201964	4053879	32					-122.2	-125.87	-129.53	-133.2	>-168				
EB-36	4199810	4053771	24.46					-91.24	-100.87	-110.51	-120.14	>-170.54				
EB-37	4197124	4054177	41.26					-83.44	-86.14	-88.84	-91.54	-154.74				
G-23	4198928	4053550	37.43					-87.57	-92.57	-97.57	-102.57	>-142.57				
G-28	4200173	4052086	36.09					-96.41	-100.74	-105.08	-109.41	>-158.91				
G-29	4201437	4052832	35.83					-111.17	-113.17	-115.17	-117.17	>-164.17				
GGWMW2	4193840	4056858	52.5	17	-42	-51		> -68								
GGWMW3	4192846	4056825	52.5	23	-47	-51		> -68								
MWG001	4197176	4059055	54		-46	-58	-64.00	-70	-96	-103	-108	> -133				
MWG002	4197175	4058357	55		-59	-62	-69.00	-76	-91	-97	-104	> -140				
SBL0013	4199584	4058732	36.4	-39	-47	-47	-90	-101	-109	-135	-144					
SBL0014	4198063	4056984	38.39	-21	-38	-47	-83	-96	-98	-104						
SBL0015	4198907	4058894	37.2	-34	-54	-60	-93	-115	-119	-127	-131					
SBL0016	4198842	4056885	35.72	-34	-53	-53	-92	-109								
SBL0019	4201224	4057883	21.34	-61	-84	-84	-101	-105	-113	-133	-141					
SBL0020	4197440	4056537	42.35	-15	-35	-63	-68.5	-72	-84	-90	-100					
SBL0021	4198037	4059262	42.7	-30	-46	-57	-74	-92	-100	-110	-115	-182				
SBL0022	4200338	4057885	32	-50	-66	-66	-98	-113	-124	-140	-149					
SBL0023	4199215	4056525	34.75	-33	-51	-51	-88	-101	-106							
SBL0024	4198585	4056524	36.44	-27	-56	-56	-92	-104	-112							
SBL0025	4201300	4059096	23.59	-51	-65	-65	-104	-112	-116	-130						
SBL0026	4200391	4056456	31.53	-58	-71	-71	-101	-124	-130							
SBL0027	4198428	4060735	40.38	-49	-79	-103	-105	-116	-122	-132	-138	-216				
SBL0028	4201141	4056416	26.75	-60	-73	-73	-109	-129	-136.00	-143.00	-150					
SBL0029	4198634	4058107	39.71	-32	-36	-36	-86	-105	-116							
SBL0030	4198030	4059899	42.22	-33	-54	-63	-82	-95								
SBL0031	4201301	4057135	23.98	-66	-73	-73	-98	-105	-115	-124	-136					
SBL0032	4199326	4060737	36.7	-57	-87	-97	-111	-120								
SBL0034	4199336	4060109	40.09	-57	-91	-97	-113	-120	-123	-130	-141					
SBL0035	4200685	4058611	28.65	-56	-69	-69	-99	-106	-114	-119	-135					
SBL0050	4198271	4058410	40.9	-30												
SBL0051	4201891	4057040	23.64	-71	-76	-76	-104	-112	-122	-126	-146					
SBL0052	4200097	4056873	33.9	-54	-78	-78	-103	-117	-121	-136	-144					
SBL0053	4200451	4055844	20.15	-54	-78	-78	-103	-112	-117	-132	-146					
SBL0054	4201078	4055866	21.1	-61	-69	-69	-109	-125	-128	-149	-156					
SBL0059	4199423	4056862	34.81	-40	-51	-51	-87	-107	-115	-131	-136					

TABLE 2-2
Hydrostratigraphic Control Points

					1	1	1	Bas	e Elevatio	n ¹ of Hydro	stratigrap	hic Unit	1	T	T	
Location	X-coordinates ²	Y-coordinates ²	Reference Elevation ¹	UBF	MBFB	MBFM	MBFC1	MBFC2	LBF1	LBF2	LBF3	Gage	GLA1	GLA2	GLA3	Lynwood
SBL0065	4198400	4056617	38.94	-21												
SBL0077	4200260	4054982	23.15	-48	-60	-60	-92	-108	-109	-119	-130	-190				
SBL0078	4197954	4058850	42.3	-32	-46	-57	-80	-90	-96	-107	-116	-182				
SBL0079	4198261	4058275	42.31	-33	-43	-50										
SBL0080	4198562	4056183	36.2	-47	-58	-58	-85	-108	-110	-116	-117	-176				
SBL0081	4199553	4057684	33.21	-46	-59	-59	-95	-104	-113	-130	-139					
SBL0084	4199556	4056522	32.72	-41	-57	-57	-89	-104								
SBL0097	4198884	4057958	36.28	-42	-47	-47	-84	-100	-106	-108						
SBL0099	4198445	4057717	39.5	-34	-43	-49	-79	-105								
SBL0101	4199100	4057244	36.79	-41	-45	-45	-80	-100	-109	-116						
SBL0103	4198993	4056528	35.4	-35	-39	-39	-70	-97	-101							
SBL0106	4199976	4056155	23.69	-49	-54	-54	-100	-108	-110							
SBL0107	4199614	4055494	29.39	-40												
SBL0108	4198515	4056928	38.52	-33	-46	-48	-83	-108	-112.67	-117.33	-122					
SBL0475	4198425	4058438	40.85	-26	-48	-56	-79.50	-103								
SBL0476	4198053	4058306	40.64	-31	-45	-56	-80.00	-104	-114	-118	-120	-180				
SBL0498	4198018	4058469	39.35	-31	-46	-55	-79.00	-103	-105	-114	-118					
SBL0499	4198329	4057715	41	-36	-39	-49	-74.50	-100	-105	-118	-120					
SBL0500	4198788	4057623	38	-35				-105	-109	-123	-131					
SBL0501	4198032	4057569	39.92	-27	-43	-52	-76.50	-101	-106	-109	-114					
SWL0060	4201259	4057095	24.95	-69				-105								
WCC-1D	4196999	4059832	50		-57	-63	-77	-87								
WCC-3D	4196831	4059937	51		-59	-68	-72	-80								
X-13DGE	4201400	4053550	30													
X-785BLACO	4191400	4054000	68	10	-7	-7	-40	-61	-61	-61	-61				-235	-285
X-794ALACO	4196100	4059441	51									-159	-185	-213	-239	-289
X-795LACO	4196530	4056700	46												-202	-252
X-808LACO	4198750	4045750	57	25	1	-23	-53	-73	-79	-89	-98	-123	-143	-164	-184	-234
X-813NLACO	4200350	4062700	35	-81	-85	-105	-115	-125	-136	-154	-171	-241	-259	-277	-295	-345
X-814DLACO	4202500	4059000	18.3	-57	-67	-73	-87	-108	-122	-137						
X-816LACO	4202220	4054000	30									-196	-211	-225	-240	-290
X-822FFLACO	4203650	4066200	27	-87	-123	-135	-155	-168	-185	-213	-237	-303	-313	-323	-333	-383
X-825LACO	4204200	4055400	18	-62	-74	-87	-130	-152	-164	-182	-200	-224	-245	-266	-286	-336
X-835ELACO	4208300	4054800	8.9	-37	-58	-81	-108	-120				-				
X-836ALACO	4206700	4051200	25	-37	-51	-51	-81	-94	-100	-109	-118	-173	-180	-188	-195	-245
XBF-18	4196366	4058108	51.35	-19	-33	-57	-75.50	-94	-96.00	-98.00	-100					-
XBF-32A	4194857	4055589	54	7	1				3 2 . 2 2	32.00						
XDA-1A	4200434	4055845	21.56	<u> </u>	1							-200	-217	-234	-250	-300
XDM-3	4198869	4056467	32	-34	1											+

TABLE 2-2

Hydrostratigraphic Co	THE OF TOWNS							Bas	e Elevatio	n ¹ of Hydro	ostratigrapl	nic Unit				
Location	X-coordinates ²	Y-coordinates ²	Reference Elevation ¹	UBF	MBFB	MBFM	MBFC1	MBFC2	LBF1	LBF2	LBF3	Gage	GLA1	GLA2	GLA3	Lynwood
XEB-01	4196227	4057561	49.1	3	-19	-41	-53	-74	-79	-89	-90	-152				
XEB-03	4197791	4057207	40.87	-14	-38	-49	-78	-90	-96	-100	-112	-174	-183	-192	-200	-250
XEB-04	4197706	4056869	42.7	-16	-32	-43	-70	-81	-90	-96	-106	-167	-175	-182	-189	-239
XEB-05	4197394	4056505	41.5									-158	-164	-171	-178	-228
XEB-06	4196937	4056497	44	-8	-29	-43	-60	-80	-84	-90	-96	-150	-157	-165	-172	-222
XEB-08	4196877	4057820	49.28	-2	-18	-47	-71	-88	-90	-95	-99	-171	-177	-183	-189	-239
XEB-09	4199639	4056482	31.14	-40	-56	-56	-84	-106	-112	-130	-140	-191	-203	-216	-228	-278
XEB-10	4198999	4056480	35.4	-40												
XEB-11	4198585	4055652	37.8	-26	-41	-41	-71	-84	-91	-102	-113	-173				
XEB-12	4199599	4055474	31	-38	-43	-49	-84	-100	-106	-125	-149	-189	-199	-209	-219	-269
XEB-13	4200059	4054027	25	-37	-50	-50	-81	-97	-103	-113	-123	-185	-192	-198	-205	-255
XEB-14	4198540	4054420	31.97	-36	-48	-59	-79	-93	-97	-104	-110	-168	-172	-176	-180	-230
XEB-15	4197240	4054950	40.54	-38	-44	-54	-69	-84	-86	-88	-89	-159	-164	-168	-172	-222
XEB-16	4199540	4052130	25.34	-23	-43	-59	-77	-90	-91	-94	-99	-153	-169	-186	-203	-253
XEB-17	4194718	4052814	37.12	-21	-33	-33	-58	-70	-77	-84	-91	-155	-167	-180	-193	-243
XEB-2A	4197200	4056890	44.6	-3	-28	-59	-65	-81	-86	-90	-95	-155	-163	-171	-178	-228
XG-08	4197974	4055531	23.87	-44	-51	-51	-67	-99	-102	-105	-109					
XG-10	4196470	4057900	49.87	-4	-33	-46	-68	-83	-88	-97	-105					
XG-12	4198949	4056036	26.95	-40	-57	-77	-97	-108	-111	-117	-122					
XG-16	4197573	4055518	38.17	-42	-52	-52	-67	-93	-96	-100	-105					
XL-1MO	4192336	4055705	54	-16								-133	-150	-183	-216	-266
XLW-01	4196897	4057220	45.5	5	-25	-64	-76.5	-85	-87	-91	-96	-164	-169	-174	-179	-229
XLW-03	4197827	4057929	41.42	-25	-47	-63	-80	-92	-97	-106	-117	-172	-179	-187	-195	-245
XMW-01T	4197965	4058543	41.77	-29												
XMW-02T	4197845	4058641	42.76	-27												
XMW-03	4196+252	4057308	47.41	1	-19											
XMW-16	4196283	4055732	42.01	-1	-13	-17										
XMW-22	4196753	4055480	41.12	-2	-27											
XMW-29	4198349	4056813	39.23	-32												
XMW-30	4198216	4056157	37.93	-17												
XP-1	4199266	4056202	33.4	-34												
XP-3	4199902	4056422	29.78	-46												
XPZ-300MO	4191073	4056771	55	-34	-55	-55	-76	-86	-86	-86	-86	-140	-174	-209	-243	-293
XS-302	4196835	4057286	48	4	-16	-61	-73	-81								

¹ Elevations are in feet with respect to National Geodetic Vertical Datum of 1929 (NGVD 29).

² X and Y coordinates are based on California State Plane Zone 7, North American Datum (NAD), 1927. Italicized values are interpolated or extrapolated from nearby data.

The top surface of the model was also updated with the 2006 baseline water level data. Similar to the previous modeling efforts, such as initial calibration and data gap analysis, the top surface of the model was assumed to be constant (i.e., it was assumed that the top aquifer is confined). As discussed in the Work Plan Amendment for the Development of the Remedial Design Model and Optimization of the Remedial Wellfield (CH2M HILL, 2006a), this assumption was required when PEST was used in conjunction with MODFLOW, because PEST could not be used efficiently if any model cells became unsaturated (i.e., became dry cells). However, simulation of an unconfined top aquifer using MODFLOW would most likely result in the occurrence of dry cells. While alternative approaches for solving this issue using other available model codes would result in significant cost and time increases for the modeling effort, the assumption of confined conditions for the water table aquifer was not expected to impact the outcome of the wellfield optimization (CH2M HILL, 2006a). This is because the remedial actions (i.e., remedial pumping and injection) will primarily target the deeper aquifers such as the MBFC and Gage aquifers (i.e., model layers 4, 5, and 9), while the confined conditions will be assumed for layers 1 and 2. Consequently, an approximation of confined conditions for the water table aquifer was considered to be acceptable.

2.5 Hydrogeologic Properties

Aquifer hydraulic conductivity is a key parameter required in the flow modeling. Initial ranges of hydraulic conductivities were estimated based on aquifer pumping tests and laboratory tests conducted during the RIs. In addition, nine aquifer extraction and four injection tests were performed by Montrose during the RD investigations. The pilot tests were generally performed at flow rates similar to expected operational remedial wellfield flow rates. A comprehensive set of water level response measurements was collected during the pilot tests from a large number of monitoring wells screened in different HSUs. Detailed discussion of the pilot tests is presented in the Pilot Extraction and Aquifer Response Test Completion Report (H+A, 2008). These tests provided the most comprehensive data pertaining to hydraulic conductivities and storage coefficients of the HSUs beneath the Dual Site. The hydrogeologic properties of the HSUs were determined based on the model calibration to the pilot test data (see Section 3.1.3.3).

2.6 Groundwater Budget

The groundwater budget components of the model include recharge and discharge components. The recharge components include groundwater inflow into the modeling domain from the upgradient areas and surface recharge. The regional inflow was accounted for through the use of GHB conditions. The surface recharge within the modeling domain includes infiltration of rainfall water, landscape irrigation, and leakage from sewer lines and the Dominguez Channel. The surface recharge was a calibration parameter and was estimated during the model calibration (see Section 3). The rates of total surface recharge were assumed to range from 0.01 to 4 inches per year (in./yr), which is reasonable considering that some areas get more infiltration of rainfall and irrigation water, while other paved areas have very limited recharge.

The only known groundwater extraction wellfield within the model domain is located at the Mobil Refinery Superfund site. The coordinates and extraction rates of the Mobil wells are presented in Table 2-3. The locations of Mobil wells are also shown in Figure 2-1.

TABLE 2-3 Mobil Refinery Extraction Wells

Well Name	Easting (feet)	Northing (feet)	Extraction Rate (gpm)	Model Layers
Mobil-2	4190982	4056735	146.8	1 – 9
Mobil-3	4191265	4056735	132.7	1 – 9
Mobil-4	4191548	4057301	200.6	1 – 9
Mobil-6	4192538	4055462	130.6	2 – 9

2.7 Contaminant Distributions

As further discussed in Section 3, all available chlorobenzene, benzene, and p-CBSA concentrations, including sampling results for the period of 1985 through 2006, were used for model calibration. The 2006 baseline data were used as initial conditions for the contaminant concentrations for the remedial wellfield optimization runs (see Section 4). The modeled initial concentrations in the water table, MBFC, and Gage aquifers are shown in Figures 2-5 through 2-7 for the chlorobenzene, benzene, and p-CBSA plumes, respectively.

The distribution of TCE was characterized during the RI and RD activities based on the data collected by Montrose and Shell, and available data collected by others including Boeing, International Light Metals, APC, and PACCAR. The dissolved distribution of TCE is shown in Figure 2-8. However, the contaminant distribution and sources for the TCE plume were not sufficiently characterized for solute transport simulations of this constituent. Consequently, only advective transport of TCE (i.e., particle tracking) was simulated as part of these modeling activities to optimize containment of the TCE plume (see Section 4.1.1.3).

Initial concentrations for the chlorobenzene, benzene, and p-CBSA plumes in the LBF (model layers 6 through 8) were assumed to be transitional between the concentration distributions in the overlying MBFC and underlying Gage aquifers. The assumed distributions in the middle aquitard layers were calculated as the geometric mean of the bounding aquifers. The distributions in the upper and lower aquitard layers were subsequently calculated as the geometric mean of the middle aquitard layer and the upper or lower bounding aquifers, respectively. Initial concentrations for model layer 3, which is composed of both the Middle Bellflower B-Sand (MBFB) aquifer and the MBFM aquitard, were set equal to the water table concentrations used in model layers 1 and 2. Model layers 10 through 13 were assigned concentrations of zero.

2.8 Source Terms

The source terms for the benzene, chlorobenzene, and p-CBSA plumes incorporated into the numerical model are briefly discussed below.

2.8.1 Benzene Source Terms

Locations and strengths of benzene sources within the Dual Site were initially developed based on multiple lines of evidence obtained during the RI, including: (1) the historical facility layout; (2) known or inferred former chemical processes; (3) chemical characterization of light nonaqueous phase liquid (LNAPL); (4) groundwater analytical data; (5) shallow and deep soil-gas data; (6) subsurface soil investigations and soil analytical data; and (7) anecdotal information from former facility operation personnel and post-facility construction files. As discussed in the JGWFS (CH2M HILL, 1998), the sources of benzene within the Dual Site were identified as areas where LNAPL is found or suspected in the subsurface, which are determined to be continuously supplying benzene and other LNAPL-related contaminants to groundwater. The benzene sources were further assessed and revised during the RD investigations to account for the 2006 baseline data and additional site characterization data including the TCE and benzene data acquisition activities.

It was assumed in the numerical model that the dissolved benzene concentrations in the source areas do not change with time (i.e., the concentrations are constant because the mass of dissolved contaminants that migrates away from LNAPL sources with groundwater flow is replenished by new mass dissolving from LNAPL). The benzene source terms including location (model cell), depth (model layer), and initial concentration are presented in Table 2-4 and shown in Figure 2-9.

Initial source term concentrations in each HSU were estimated from 2006 baseline monitoring data and historic benzene concentrations at these locations. These values were adjusted during model calibration to achieve a match between measured and simulated concentrations (see Section 3).

Please note that the results of groundwater sampling performed by Shell in 2008 (after the model calibration had been completed) were not incorporated into the model. These results indicated that the modeled benzene sources in the MBFC, near the waste pit source area, may be somewhat overestimated. This is because the 2008 sampling data for MBFC wells SWL0040 and XBF-13 located in this area indicated that benzene concentrations in this area were relatively low compared to the historical data for these locations (URS, 2008).

2.8.2 Chlorobenzene Source Terms

The dense nonaqueous-phase liquid (DNAPL) sources of chlorobenzene at the Montrose property were also incorporated in the numerical model of the Dual Site. Similar to the benzene sources, these sources were simulated as constant-concentration source terms based on the assumption that the mass of dissolved chlorobenzene that migrates downgradient from the DNAPL source with groundwater flow is replenished by new mass dissolving from DNAPL. Constant-concentration chlorobenzene source terms were specified for the model cells that most closely coincide with the DNAPL distribution. These cells encompass a 400- by 400-foot area that extends from the water table downward through the Gage aquifer, at model rows 41 through 44, and columns 61 through 64 (Figure 2-9). This assumed source-term depth was based on (1) the presence of DNAPL in the water-table units, (2) on the indirect evidence of DNAPL in the form of elevated concentrations of chlorobenzene and dichlorodiphenyltrichloroethane (DDT) in soil samples at the bottom of the MBFC, and (3) elevated chlorobenzene concentrations in the Gage aquifer (CH2M HILL, 1998).

The source term concentrations in each HSU were estimated from 2006 baseline monitoring data and historic chlorobenzene concentrations at these locations. These values were adjusted during model calibration to achieve a match between measured and simulated concentrations (see Section 3 for initial and calibrated values of the chlorobenzene sources).

2.8.3 p-CBSA Source Terms

Sources of p-CBSA also were simulated as constant-concentration cells in the area with the highest p-CBSA concentrations, which coincides with the DNAPL area. Constant-concentration sources for p-CBSA were assigned to the same cells that were utilized for chlorobenzene constant-concentration sources (Figure 2-9).

The source term concentrations in each HSU were estimated from 2006 baseline monitoring data and historic chlorobenzene concentrations at these locations. These values were adjusted during model calibration to achieve a match between measured and simulated concentrations (see Section 3 for initial and calibrated values of the p-CBSA sources).

2.8.4 TCE Sources

As discussed above, the contaminant distribution and sources for the TCE plume are not sufficiently characterized for solute transport simulations of this constituent. Consequently, the solute transport of TCE was not simulated as part of these modeling activities. However, advective transport of TCE (i.e., TCE migration with groundwater flow) from the source areas was evaluated to design the containment of TCE sources in accordance with the requirements of the ROD. Consequently, the approximate locations of the TCE sources were identified in the model through interpretation of available groundwater analytical data collected by others and available from agency files, as well as based on data collected as part of the Montrose and Del Amo data acquisition activities. The TCE source located at the PACCAR and APC facilities was considered for the design and optimization of the remedial wellfield, and is shown with interpreted TCE concentration contours in Figure 2-9.

2.9 Transport Parameters

The parameters required in the MT3DMS transport simulations include effective porosity, bulk density, dispersivity, retardation coefficient, and intrinsic biodegradation half-life. Each of these parameters is briefly discussed below.

2.9.1 Bulk Density and Porosity

Initial values of bulk density and porosity were obtained from laboratory tests on samples collected at the Dual Site and summarized in Appendix B of the JGWFS (CH2MHILL, 1998). Measured bulk density ranged from 1,100 to 2,600 kilograms per cubic meter (kg/m³) with an average of 1,720 kg/m³. Measured total porosity ranges from 36.5 percent to 41.8 percent using soil samples beneath the former Del Amo property. Physical tests conducted as part of the MW-20 pilot program showed that effective porosity ranges from 34.1 percent to 50.4 percent. Samples collected at the Montrose property indicated that total porosity ranges from 33.7 percent in the Lynwood aquifer to 52.1 percent in the MBFM. The variation in measured porosity can be attributed to soil heterogeneity and different sampling and testing procedures.

TABLE 2-4
Renzene Source Terms

Benzene S	Source Terms	UBF (Laver 1)								ı				1				
			UE	BF (Layer 1)			MB	FB (Layer 2)			MBI	FM (Layer 3)			MBFC	(Layers 4 and 5)		
Source Area	Description	No. of Cells	Cell Locations (row/columns)	Initial Benzene Concentration (µg/L)	Calibrated Benzene Concentration (µg/L)	No. of Cells	Cell Locations (row/columns)	Initial Benzene Concentration (µg/L)	Calibrated Benzene Concentration (µg/L)	No. of Cells	Cell Locations (row/columns)	Initial Benzene Concentration (µg/L)	Calibrated Benzene Concentration (µg/L)	No. of Cells	Cell Locations (row/columns)	Initial Benzene Concentration (µg/L)	Calibrated Benzene Concentration (µg/L)	
2	MW-20 NAPL Area	4	45/79, 80 46/79, 80	1,200,000	1,202,000	4	45/79, 80 46/79, 80	1,279,000		0				0				
	Styrene finishing/ benzene purification area	4	50/83, 84 51/83, 84	140,000	140,000	0				0				0				
5	VOC tank farm	13	48/80 49/78, 79 50/77, 78 51/76, 77 52/75, 76 53/75, 76 54/74, 75	44,000	44,000		48/80 49/78, 79 50/77, 78 51/76, 77 52/75, 76 53/75, 76 54/74, 75	44,000	44,030	0				0				
6	Ethylbenzene Production Area No. 1	10	53/78, 79, 80 54/78, 79, 80 55/78, 79, 80	275,000	275,000		53/78, 79, 80 54/78, 79, 80 55/78, 79, 80	275,000	275,000		53/78, 79, 80 54/78, 79, 80 55/ 78, 79, 80	275,000	276,200	4	54/79, 80 55/79, 80	190,000	344,500	
7	Ethylbenzene Production Area No. 2	3	55/83 56/82, 83	42,000	42,000	0				0				0				
8	Utility Tanks	5	55/71, 72 56/71, 72 57/70	300,000	335,700		55/71, 72 56/71, 72 57/70	300,000	274,700	0				0				
9	Waste Pit Area	14	61/71 62/71, 72 63/71, 72, 73 64/72, 73, 74 65/73, 74, 75 66/74, 75	300,000	420,300		61/71 62/71, 72 63/71, 72, 73 64/72, 73, 74 65/73, 74, 75 66/74, 75, 76 67/75, 76, 77 68/76, 77 69/76	80,000	79,040		61/71 62/71, 72 63/71, 72, 73 64/72, 73, 74 65/73, 74, 75 66/74, 75, 76 67/75, 76, 77 68/76, 77 69/76	80,000	80,060	4	68/75, 76 69/75, 76	49,000	64,900	
10	Laboratory and Pipelines	14	73/93, 94, 95 74/92, 93, 94, 95 75/91, 92, 93, 94 76/91, 92, 93	260,000	260,000	0				0				0				
11	Benzene Pipeline	4	75/84, 85 76/84, 85	600,000	754,000	0				0				0				
21	Jones - B	4	42/53, 54 43/53, 54	27,000	27,000	4	42/53, 54 43/53, 54	27,000	27,000	0				0				
23	Panhandle Area	12	51/67, 68 52/67, 68 53/65, 66, 67, 68 54/65, 66, 67, 68		3,000		51/67, 68 52/67, 68 53/65, 66, 67, 68 54/65, 66, 67, 68		3,000	0				0				

TABLE 2-4
Benzene Source Terms

			UE	BF (Layer 1)		MBFB (Layer 2)					МВІ	FM (Layer 3)		MBFC (Layers 4 and 5)				
Source Area	Description	No. of Cells	Cell Locations (row/columns)	Initial Benzene Concentration (µg/L)	Calibrated Benzene Concentration (µg/L)		Cell Locations (row/columns)	Initial Benzene Concentration (µg/L)	Calibrated Benzene Concentration (µg/L)	No. of Cells	Cell Locations (row/columns)	Initial Benzene Concentration (µg/L)	Calibrated Benzene Concentration (µg/L)		Cell Locations (row/columns)	Initial Benzene Concentration (µg/L)	Calibrated Benzene Concentration (µg/L)	
24	P-1 NAPL	4	69/71, 72 70/71, 72	3,100	3,100	4	69/71, 72 70/71, 72	3,100	3,100	0				0				
34	Montrose	4	49/61, 62 50/61, 62	3,000	3,000	4	49/61, 62 50/61, 62	3,000	3,000	4	49/61, 62 50/61, 62	3,000	3,000	4	4/61, 62 50/61, 62	60	60	
35	ASTs	4	59/77, 78 60/77, 78	180,000	180,000	4	59/77, 78 60/77, 78	180,000	223,100	0				0				

Notes:

VOC - volatile organic compound

AST – aboveground storage tank

However, the laboratory values of total porosity do not directly correspond to the effective porosity of aquifer materials, which controls contaminant migration. This is because effective porosity is usually a fraction of the total porosity that is available for transporting water through the aquifer and excludes the fraction of pores that are too small to hold water, or those that are not interconnected. Therefore, effective porosity of aquifer material is generally lower than that obtained in the laboratory from soil samples. An effective porosity of 5 to 20 percent was assumed for the transport simulations of the RD model. These values are lower than those measured in core samples, but are within accepted ranges found in hydrogeologic literature. The values of porosity were further adjusted during model calibration to match the measured and simulated water levels and contaminant concentrations (see Section 3 for the porosity values by HSU).

2.9.2 Retardation and Distribution Coefficients (Kd)

The retardation coefficient represents the process of sorption and desorption of contaminants onto the solid grains of the subsurface media. This process acts to "retard" or slow the average linear velocity of contaminants migrating in groundwater. The retardation factor was calculated by MT3DMS using the site-specific values of bulk density and distribution coefficient (Kd).

Chlorobenzene Kd was allowed to range from 0.001 to 6 milliliters per gram (ml/g.), based on field and literature data. Benzene Kd was fixed at values ranging from 0.002 to 0.32 ml/g, based on field data and literature values. Retardation factors for both benzene and chlorobenzene were calculated by MT3DMS from field-measured bulk density values and Kd. The retardation factors were further adjusted during model calibration to match measured and simulated contaminant concentrations (see Section 3).

It was assumed for the purposes of this modeling effort that the retardation of p-CBSA is equal to zero, because p-CBSA is a conservative constituent and its transport is not significantly affected by sorption.

2.9.3 Dispersivity

Dispersivity is another transport parameter that was considered in the development and calibration of the numerical model. Dispersion of contaminants dissolved in groundwater results from different velocities of groundwater at a scale of individual soil particles and pore spaces that affect the contaminant migration. The MT3DMS solute transport model numerically simulates this process by solving governing solute concentration equations. A dispersion coefficient is used in these solute concentration equations to characterize the effect of dispersion on the contaminant distribution in groundwater. The amount of dispersion used in the model is characterized by the parameter of dispersivity. Dispersivity was specified in the longitudinal, transverse, and vertical direction relative to the direction of groundwater flow. The initial ranges of dispersivity assigned to the model were estimated from literature values. The final values were estimated in the process on model calibration. The initial ranges and calibrated values of longitudinal, transverse, and vertical dispersivity for benzene and chlorobenzene used in the RD model are presented in Section 3.

2.9.4 Intrinsic Biodegradation

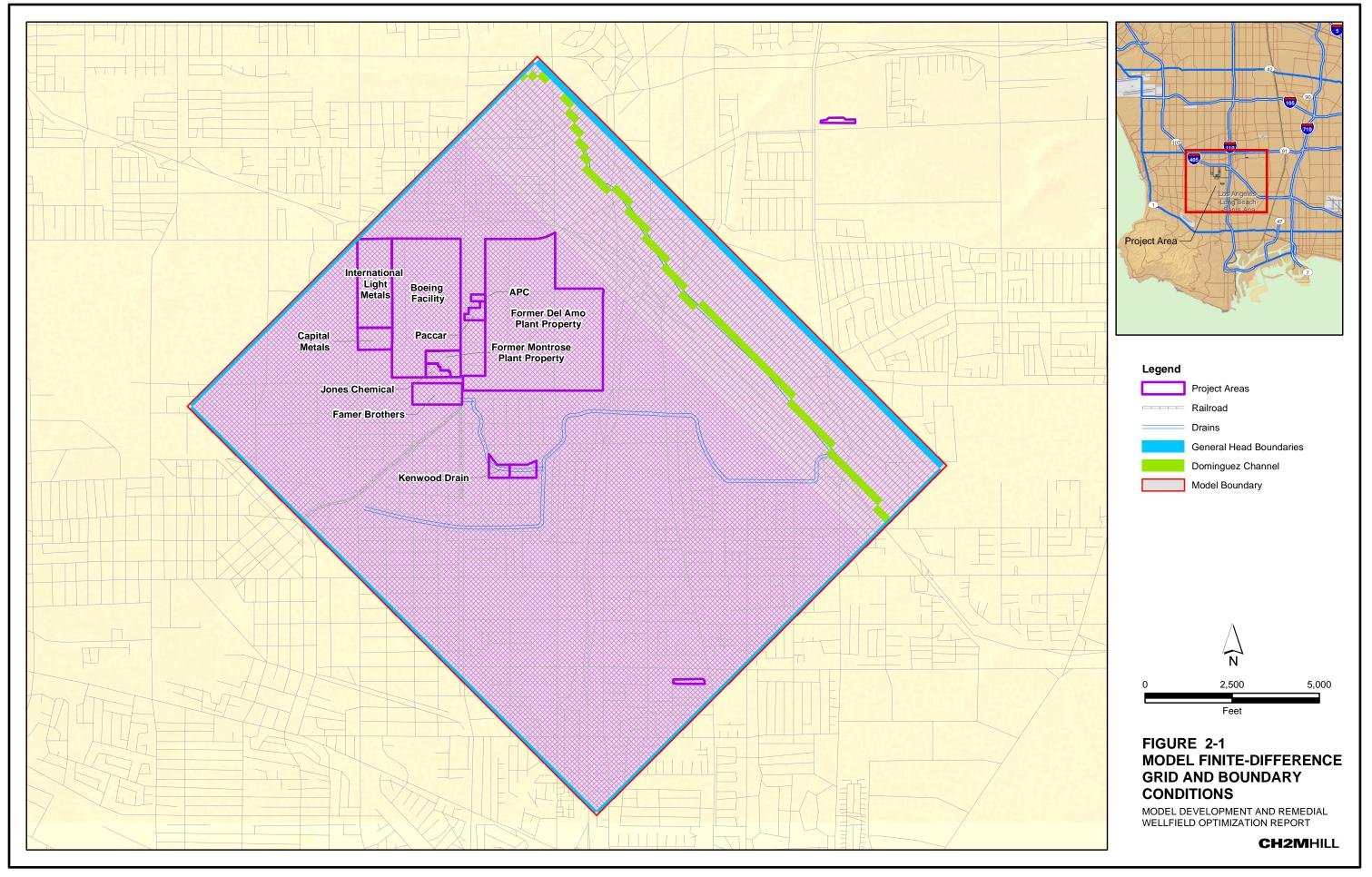
The modeling assumptions regarding intrinsic biodegradation, represented in the model by values of biodegradation half-life, are based on the discussion in the JGWFS (CH2M HILL, 1998) and recent data collected during RD including the 2004 and 2006 baseline monitoring rounds.

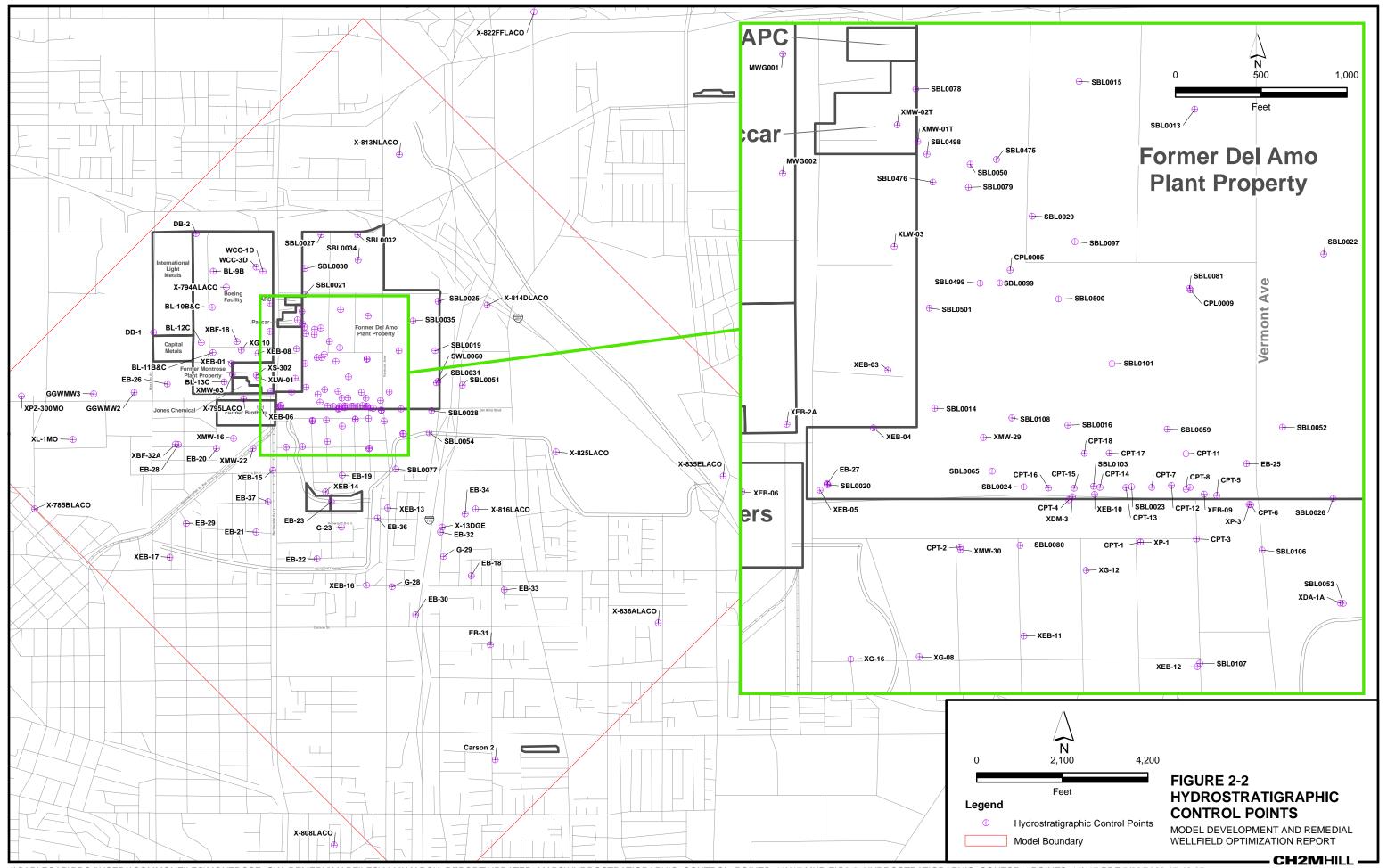
As discussed in the JGWFS and confirmed with more recent data, a number of factors indicate that intrinsic biodegradation of chlorobenzene cannot be relied upon to be a component of the chlorobenzene remedy, although it may be occurring at the Dual Site to some degree. These include the spatial characteristics of the chlorobenzene plume (especially the fact that the plume has been able to expand to its large lateral and vertical size) in conjunction with the absence of reliable data on geochemical indicators, and the lack of understanding of anaerobic biodegradation of chlorobenzene within the scientific community. Based on the above and consistent with the previous modeling efforts, no intrinsic biodegradation of chlorobenzene was assumed for the RD model.

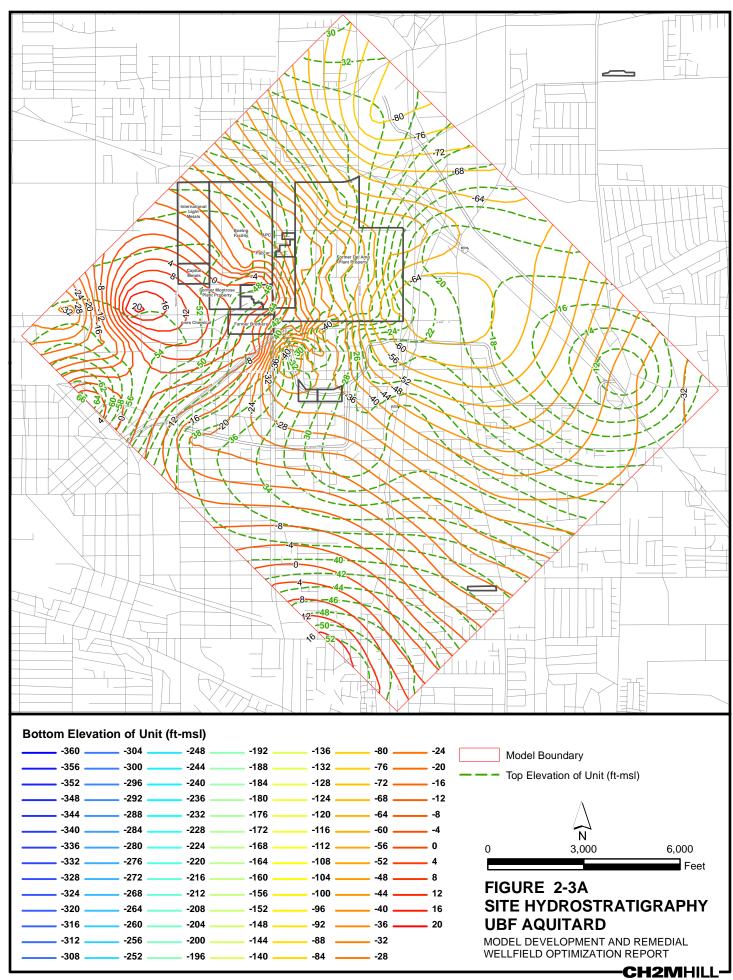
The benzene plume distribution pattern is typical for contaminants affected by biodegradation. A combination of factors such as (1) the plume distribution pattern, (2) the geochemical evidence of biological activity within the benzene plume, and (3) extensive evidence of benzene biodegradation documented in the hydrogeologic literature, indicate that intrinsic biodegradation is having a significant impact on the benzene plume, and should be considered in the remedy selection for the benzene plume.

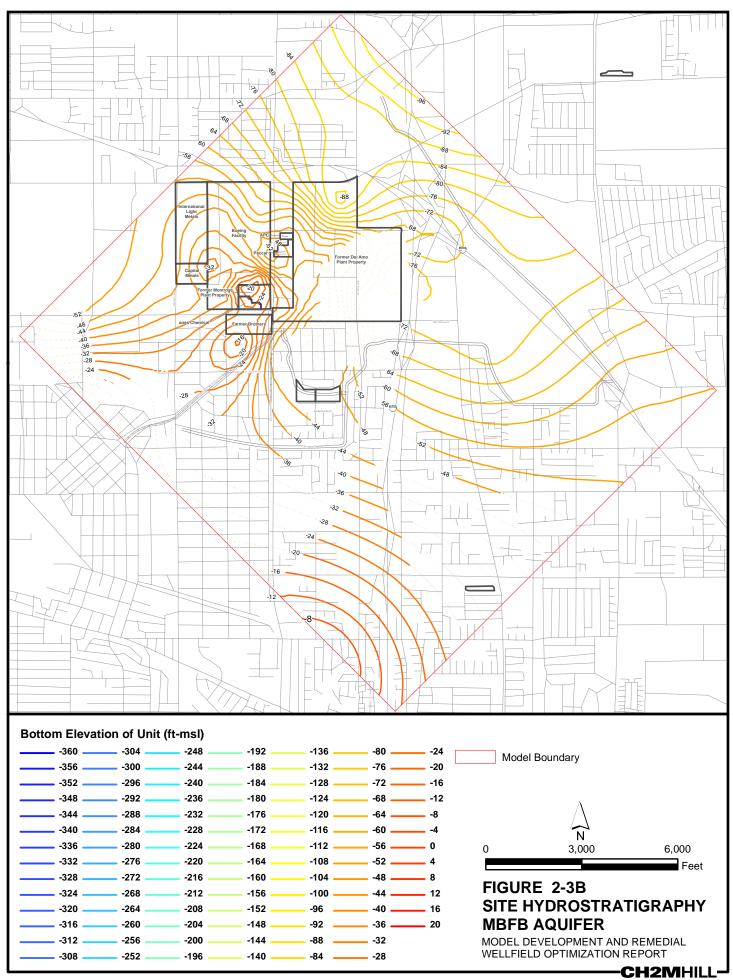
The initial model values for benzene half-life were obtained based on a range of values from literature reviews, and the site-specific focused transport study conducted during the RI/FS process (CH2M HILL, 1998). These values were further adjusted during the RD model calibration. The initial ranges and calibrated values of benzene biodegradation half-life are presented in Section 3.

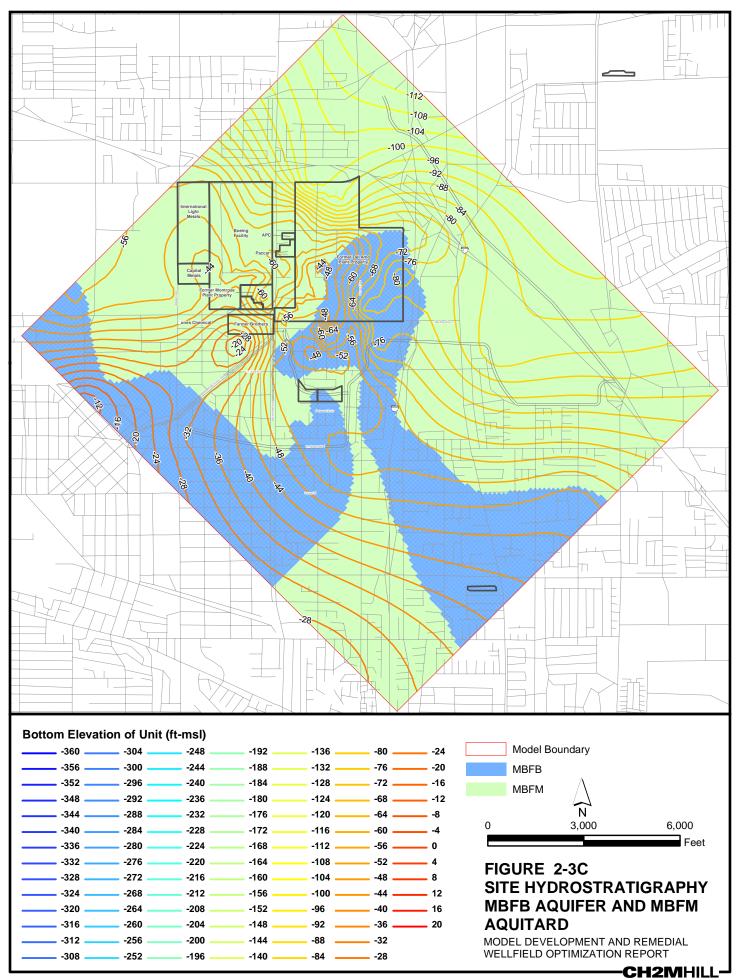
There are insufficient data to determine the degree to which intrinsic biodegradation of p-CBSA may be occurring at the Dual Site. For the purpose of this modeling effort, it is assumed that intrinsic biodegradation of p-CBSA is not occurring.

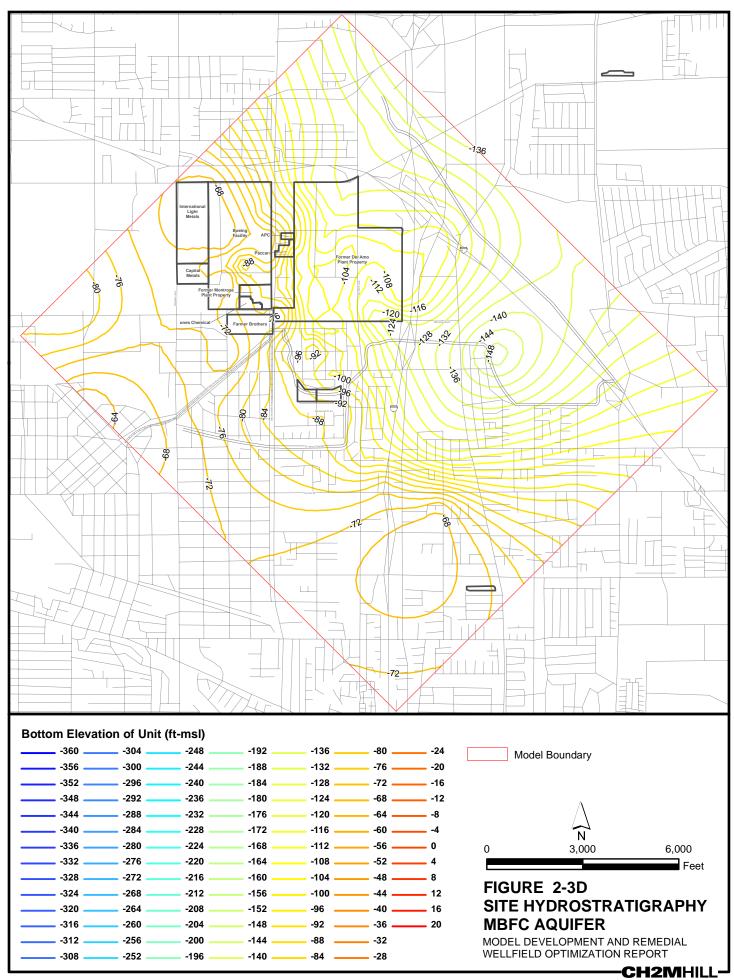


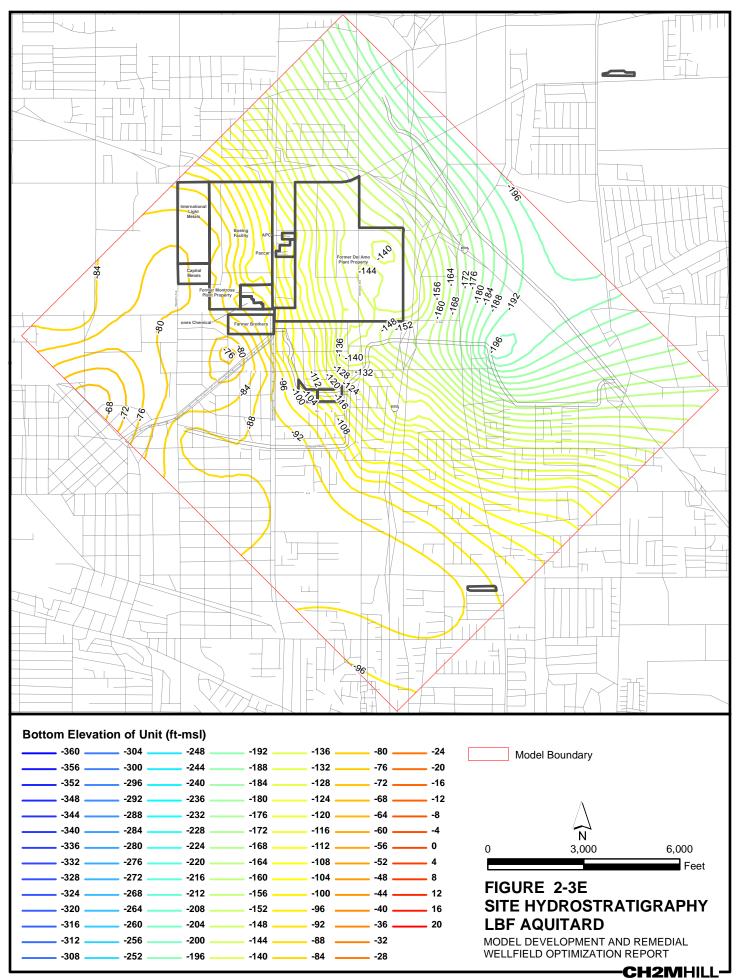


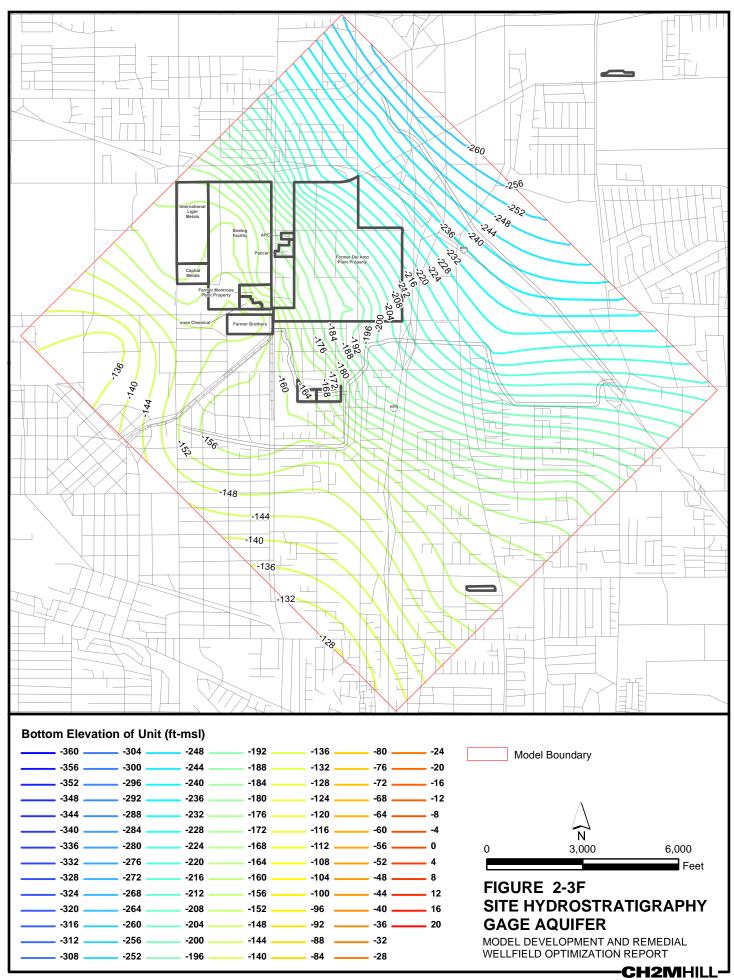


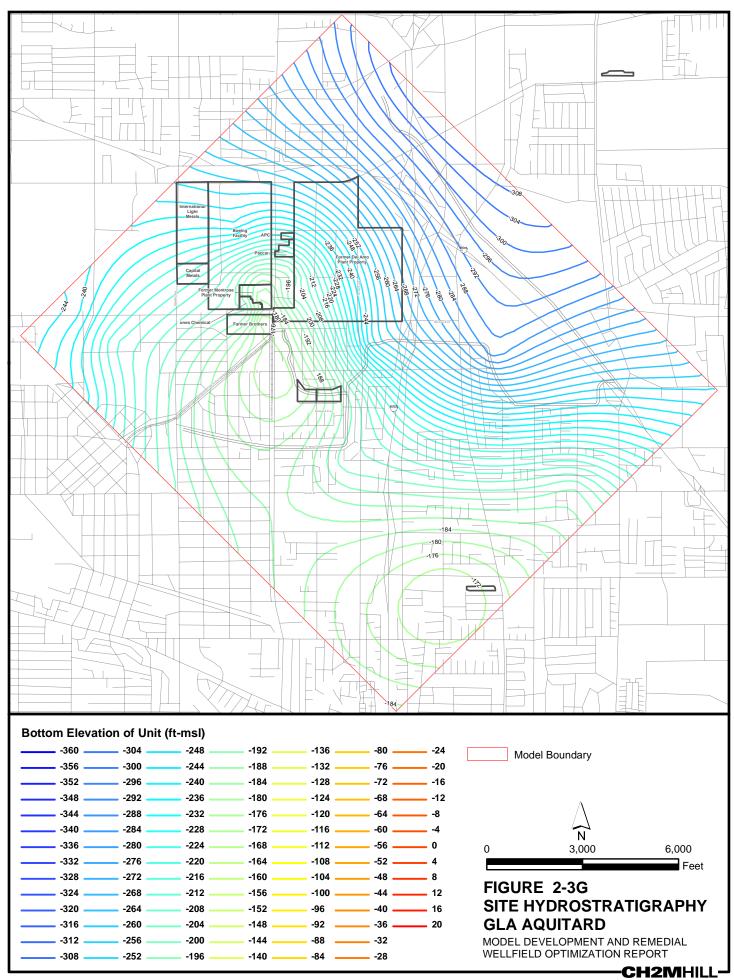


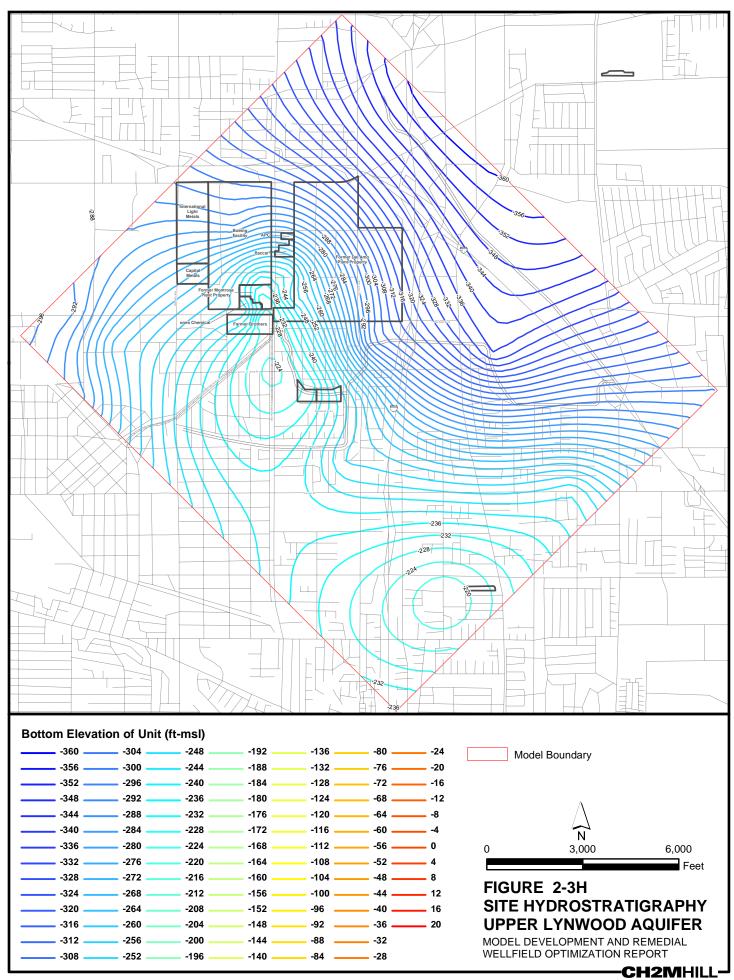


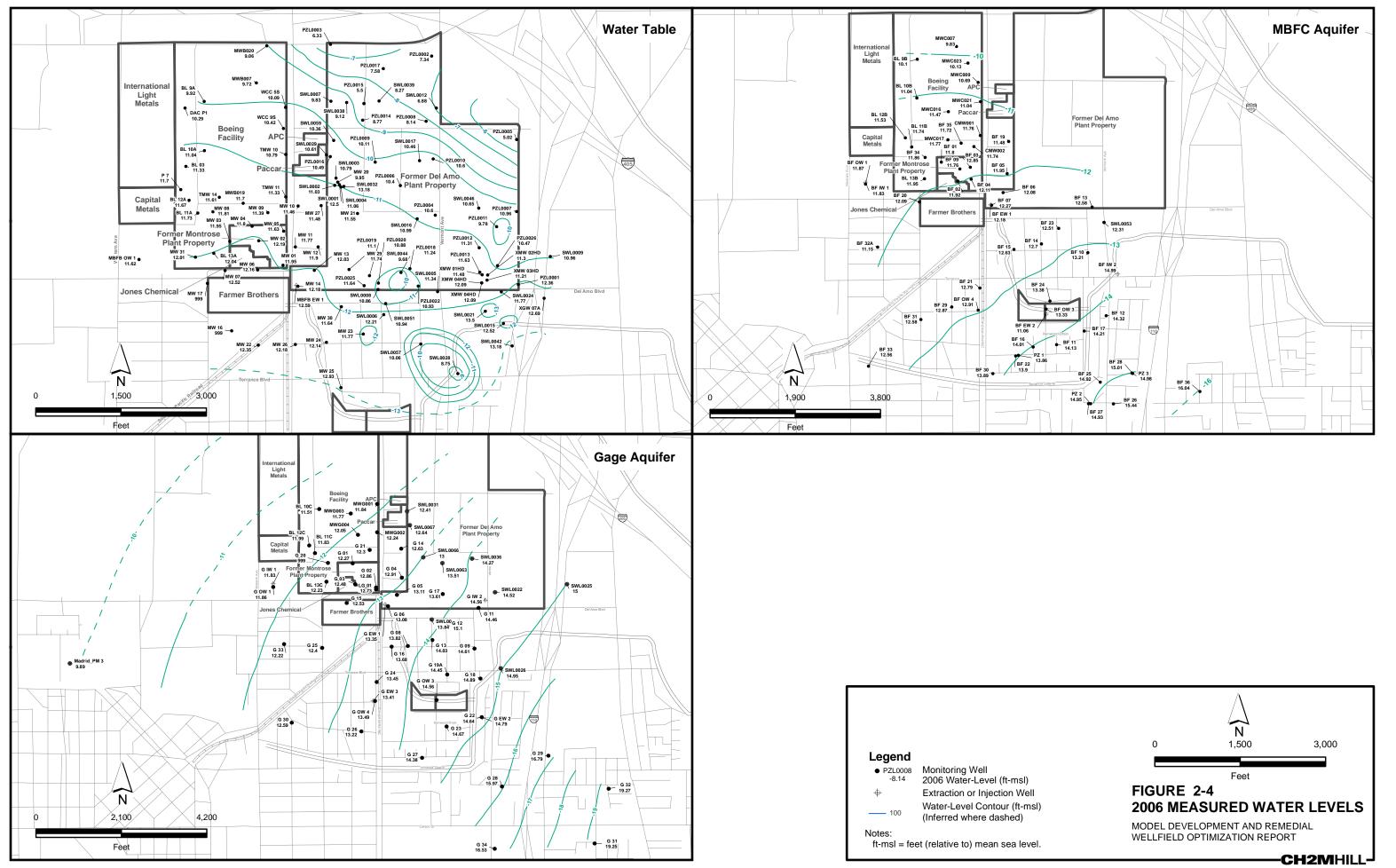


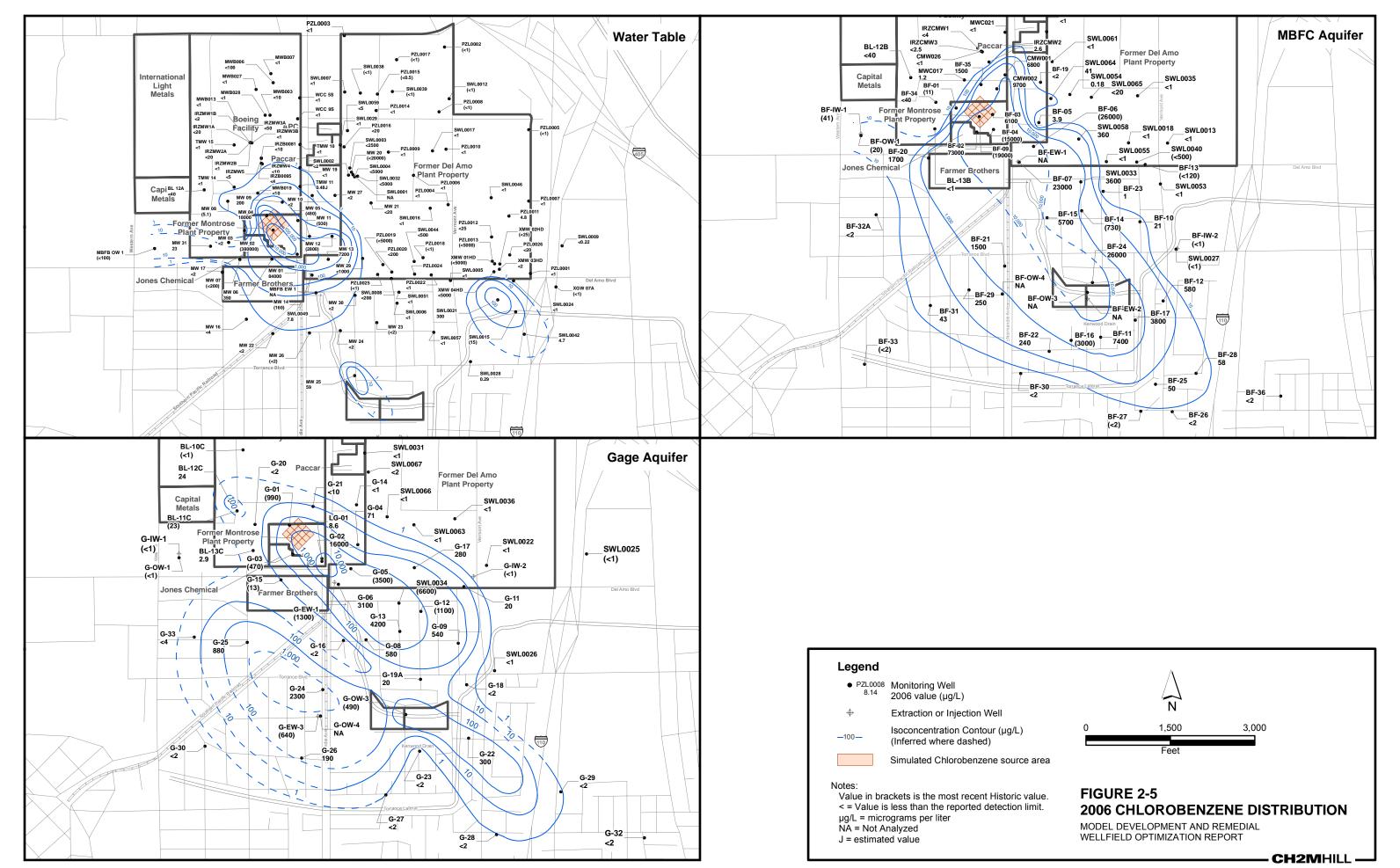


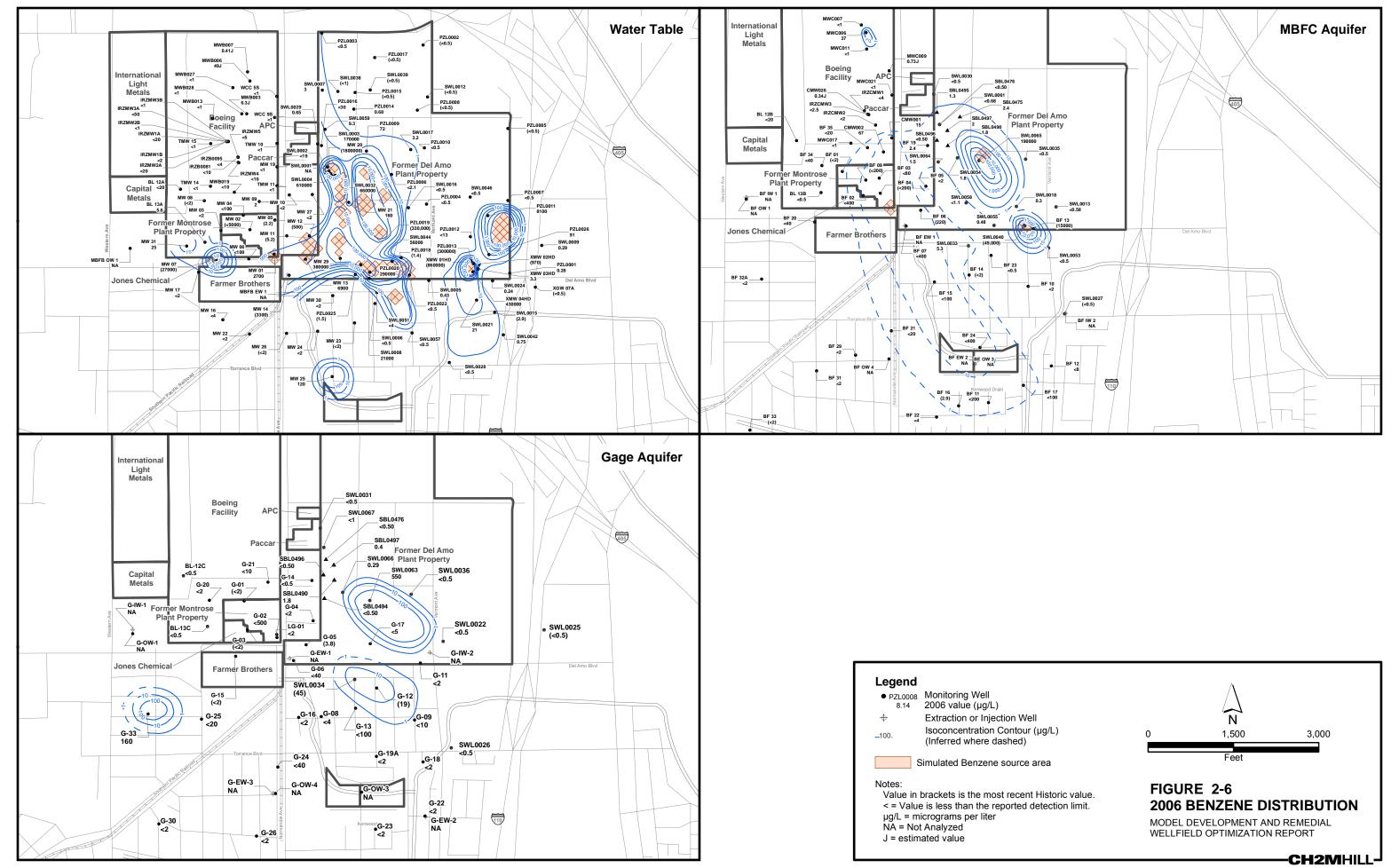


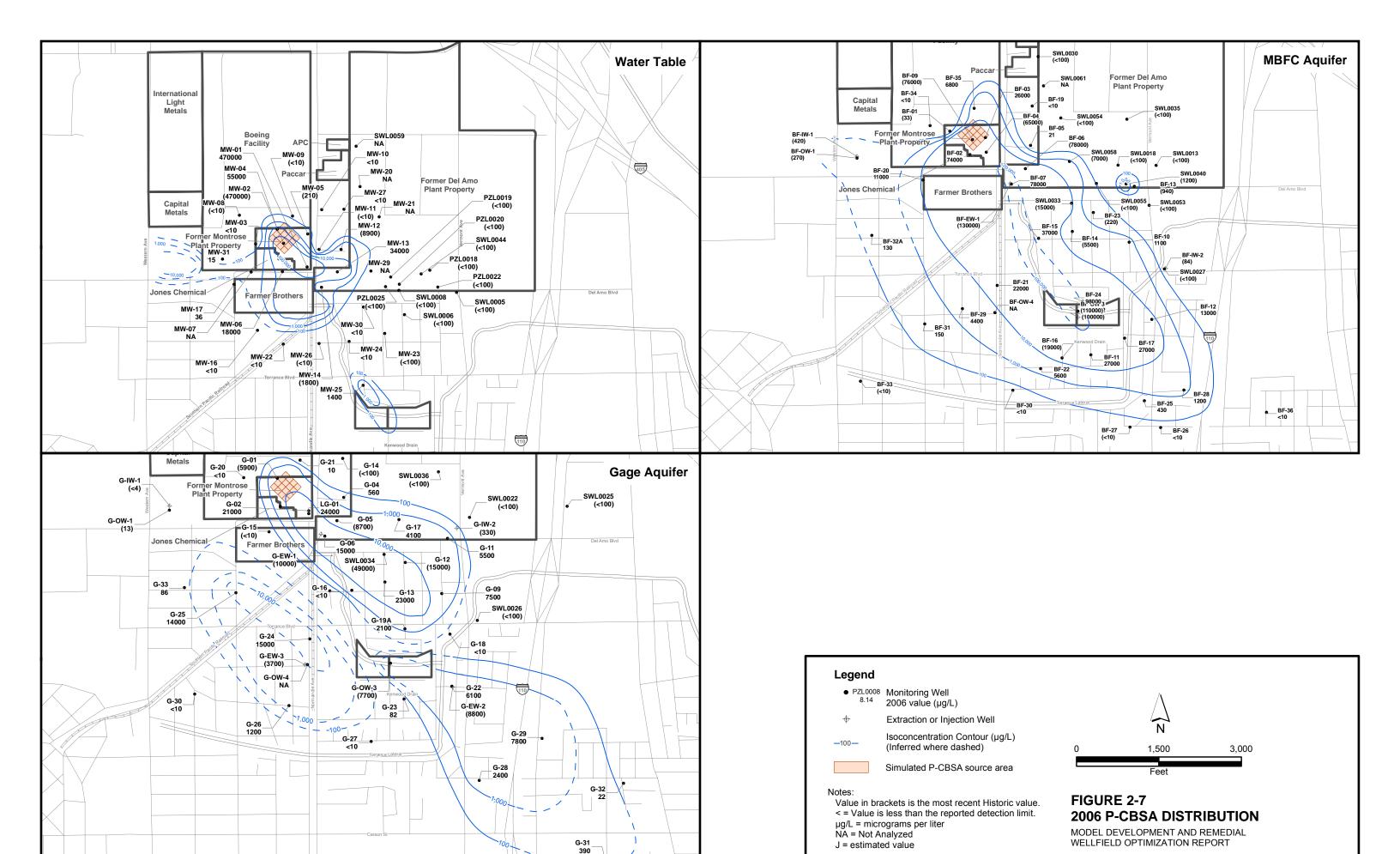




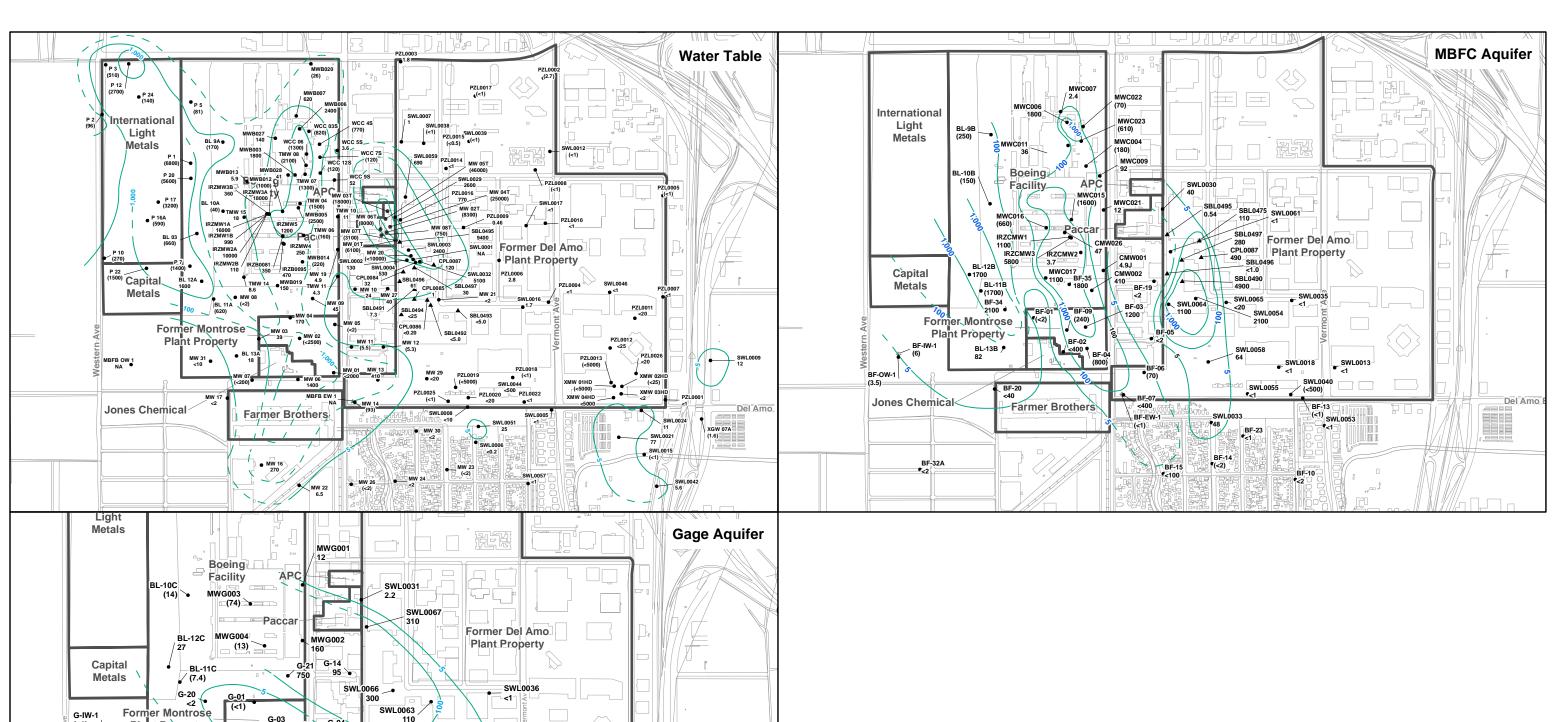


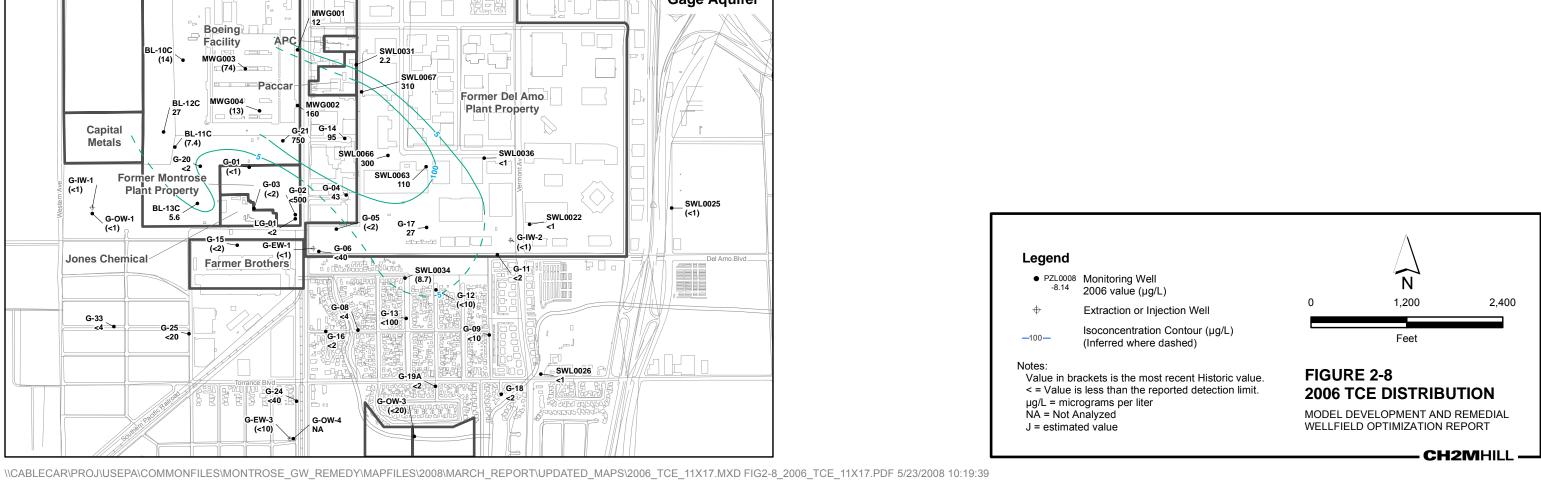






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3. Model Calibration

This section discusses the calibration of the RD model, including the calibration methodology and calibration results.

3.1 Calibration Methodology

As discussed in detail in the Work Plan for Development of the Groundwater Model for the Remedial Design (CH2M HILL, 2003) and the Work Plan Amendment for the Development of the Remedial Design Model and Optimization of the Remedial Wellfield (CH2M HILL, 2006a), the model calibration was performed using the nonlinear parameter estimation software package PEST (Doherty, 2002, 2004, 2007; Doherty and Johnston, 2003). PEST calibration was performed by automatic minimization of the objective function, which is the sum of squared residuals of the calibration targets. Calibration targets were observed or estimated parameters such as water levels and contaminant concentrations, which were supposed to be reproduced by the calibrated model. Residuals were the differences between model-simulated and observed or measured calibration targets. In the process of calibration, PEST modified calibration parameters, such as the hydraulic and transport properties of the physical system (e.g., hydraulic conductivity, porosity, dispersivity, etc.) in accordance with the prescribed parameter distribution and limits until the objective function can no longer be reduced and the best possible match was achieved between the calibration targets and the simulated results.

The groundwater flow and transport models are generally nonunique, and a similar quality of calibration can be achieved with a number of different model parameter combinations. This is because changes to certain model parameters (e.g., hydraulic conductivity) can be offset by changes to other parameters (e.g., recharge), resulting in a similarly reduced objective function, and therefore a similar quality of model calibration. Consequently, a number of models can be developed using PEST, all of which would be reasonably well calibrated and based on equally viable hydrogeologic parameters for a given physical system. These calibrated models may differ, however, with regard to predictions pertaining to the performance of the remedial wellfield, which will have a significant impact on the certainty of modeling predictions pertaining to this performance.

In order to account for the issues pertaining to the nonuniqueness of the model calibration, the following approach was used for the calibration of the RD model:

- 1. Develop the baseline calibration, which is based on the reasonable parameters and is acceptable to all parties (i.e., acceptable to EPA, Shell, Montrose, and other stakeholders) for the optimization of the remedial wellfield.
- 2. Use the baseline calibration for the development and optimization of the remedial wellfield.
- 3. Perform the wellfield failure analysis to assess the uncertainty of the model predictions pertaining to the performance of the remedial wellfield.

This section is focused on the baseline calibration of the RD model. The remedial wellfield failure analysis is discussed in detail in Section 5 of this report. Presented below is the discussion of the calibration process, parameter distribution and limits, and calibration targets for the baseline calibration.

3.1.1 Calibration Process

As discussed in detail below, the RD model was calibrated using 2006 water level data; pilot test drawdown and buildup data from the pilot extraction and injection tests; and chlorobenzene, benzene, and p-CBSA historical concentration data. The model was calibrated in a sequential fashion, gradually increasing in complexity. First, a calibration to only water levels and vertical head differences was performed. Model parameters and boundary conditions from this initial stage were used as the basis for an overall hydraulic calibration to water levels, vertical head differences, and pilot test drawdown and buildup data.

An overall hydraulic calibration run included both steady-state calibration to 2006 baseline water level data and transient flow runs for eight extraction and four injection tests. The extraction test for well MBFB-EW-1 was not simulated, due to the low yield and small magnitude and extent of hydraulic response to pumping at the well. The hydraulic parameters obtained as the result of this calibration were then used as initial and preferred values for a combined flow and transport calibration.

For the transport calibration, the transient transport run was performed for a period of 61 years, from 1945 (the assumed time of contaminant release to groundwater) through 2006 (the latest period for which the concentration data were available at the time of calibration). The initial concentrations of chlorobenzene, benzene, and p-CBSA for the calibration run were assumed to be equal to zero (i.e., the calibration run was designed to reproduce the current plumes from the time of initial release).

The calibration parameters were adjusted at each stage of increasing calibration complexity to allow for the best match between the measured and simulated results. The parameter distribution, limits and preferred values, and a set of calibration targets and weights are discussed below.

3.1.2 Parameter Distribution and Limits

As described below, the values of some model parameters were fixed (i.e., were not allowed to change in the calibration process), while others, referred to as calibration parameters, were allowed to vary to achieve the best match between the simulated conditions and calibration targets. Fixed parameters were assigned values based on field data when these data were available and on literature and professional judgment where field data were not available. Calibration parameters were estimated using PEST. These estimates were performed in accordance with the parameter distribution and limits assigned to each calibration parameter. For some parameters, which were assumed to be constant within an HSU and/or model layer, a single value was estimated per model layer or HSU. Other parameters were estimated using pilot points. As discussed in the Work Plan for Model Development (CH2M HILL, 2003), pilot points are discrete locations where PEST estimates values of the particular calibration parameter needed to match calibration targets at this

location. The values of calibration parameters at all model cells were then interpolated based on the values at the pilot points.

The parameter distribution, limits, and preferred values assumed for the baseline calibration are presented below.

Parameter Distribution

The assumptions regarding the distribution and variability of calibration parameters and values for fixed parameters for the baseline calibration are described below.

Distribution of Calibration Parameters

The assumed spatial distribution for each parameter is presented in Table 3-1 and described below.

- Horizontal hydraulic conductivity (Kh), Kh and vertical hydraulic conductivity (Kv) ratio (Kh:Kv) of upper units, recharge, and Dominguez Channel conductance were assumed to be spatially variable (i.e., were allowed to vary within HSUs).
- Storage coefficients (Sy, Ss) were assumed to be constant in each HSU, but were permitted to vary between aquifer tests. Storage coefficients were grouped together where limited information was available. For example, the same specific storage for the MBFC aquifer was used during calibration to the pilot test data in the Gage aquifer, but a different storage coefficient for the Gage aquifer was estimated for each test. This is because the Gage pilot test data provided more information regarding the storage coefficient in the Gage, than regarding the storage coefficient in the MBFC.
- Transport parameters such as porosity, dispersivity, distribution coefficient (Kd), retardation factor (R), decay rate, and source concentrations were assumed to be constant within HSUs, but were allowed to vary in different HSUs.
- GHB conductance was calculated from the calibrated hydraulic conductivity values for each GHB cell using the following equation: GHB conductance = K*L*W/M, where K is the horizontal hydraulic conductivity at a particular cell, L is the thickness of the cell, W is the size of the cell in the direction perpendicular to flow, and M is half the size of the cell in the direction parallel to flow.

As discussed in the Work Plan for Model Development (CH2M HILL, 2003), the spatial continuity targets were added to the objective function to achieve a homogeneous distribution of parameters unless suggested otherwise by field data used as calibration targets.

Variability of Calibration Parameters

The assumed transformation status and standard deviation for each model parameter is presented in Table 3-1. Fixed parameters were not estimated as part of the calibration process.

TABLE 3-1
Assumed Parameter Distribution and Transformation Status

Parameter	Spatial Distribution	Transformation Status
Porosity	Constant in each HSU	Fixed
Longitudinal dispersivity	Constant in each HSU	Log
Transverse dispersivity	Constant in each HSU	Log
Vertical Dispersivity	Constant in each HSU	Log
Chlorobenzene source concentration	Constant within source area in each HSU	Log
Chlorobenzene Kd	Constant within each layer	Log
p-CBSA source concentration	Constant within source area in each HSU	Log
Benzene source concentration	Constant within each source area in each HSU	Log
Benzene Kd	Constant within each layer	Fixed
Benzene degradation rate	Constant within each layer	Log
Riverbed conductance	Four pilot points along river length	Log
Elevation of GHB	Several pilot points along boundary in each aquifer	Fixed
Specific yield and specific storage	Constant in each HSU	Log
Recharge	Pilot points	None
Hydraulic conductivity	Pilot points within each HSU	Log
Horizontal to vertical hydraulic conductivity ratio	Pilot points within each HSU	Log

Fixed Parameters

- Values of porosity were fixed (i.e., were not allowed to change in the calibration process) to correct numerical stability problems during PEST runs.
- Values of benzene Kd were fixed at values calculated from analysis of field samples and literature values.
- Values of Kh:Kv were fixed for lower HSUs (the MBFM through Lynwood aquifer).
- Values of GHB heads were estimated based on the extrapolation of available water levels and fixed.
- Source timing was fixed.

Parameter Limits and Preferred Values

Parameter limits and preferred values for flow and transport parameters are discussed below.

Parameter Limits for Flow Parameters

- Kh was allowed to range within plus/minus two standard deviations (log-transformed) of the geometric mean of available aquifer test data, or within plus/minus 1.5 orders-of-magnitude of values estimated during previous investigations at the Dual Site. Initial Kh values and ranges in the MBFC and Gage aquifers were derived from preliminary analysis of extraction and injection pilot test data.
- Kh:Kv ratio was allowed to range from 1:1 to 100,000:1 in the UBF and MBFB, and was fixed at 10:1 in lower units (i.e., in the MBFM through Lynwood aquifer). The wide range of permitted values in the upper units could have been reasonably constrained to a smaller range, but early PEST runs showed no tendency toward extreme values.
- Recharge was allowed to range from 0.01 to 4 in./yr, which is reasonable for Dual Site conditions.
- Specific yield and specific storage were allowed to range from 1x10-9 to 0.3, which ranges from confined behavior and rapid aquifer response at the low end, to unconfined behavior and slow aquifer response at the high end of this range.
- Dominguez Channel conductance was allowed to range within an order-of-magnitude of values estimated from the channel geometry and previous investigations at the Dual Site.
- GHB heads were assigned using four to seven pilot points per aquifer layer including one point at each model corner (i.e., four points), and additional points at the locations where water-level data were available near the boundary. GHB heads for aquitards were assigned as averages of heads in the underlying and overlaying aquifers. For example, the GHB head in Layer 11 of the GLA was calculated as the average of head in the Gage aquifer (Layer 9) and in the Lynwood aquifer (Layer 13). GHB head in GLA Layer 10 was then calculated as the average of heads in Layers 9 and 11.

Parameter Limits for Transport Parameters

- Porosity was fixed at values ranging from 5 to 20 percent on the basis of field data.
- Longitudinal dispersivity (D_L) was allowed to range from 0.1 to 1,000 feet, based on the scale of the plume.
- Transverse (D_T) to longitudinal dispersivity ratio was allowed to range from 0.001 to 1, based on literature estimates.
- Vertical (D_Z) to longitudinal dispersivity ratio was allowed to range from 1x10-6 to 1, based on literature estimates.
- Chlorobenzene Kd was allowed to range from 0.001 to 6 ml/g, based on field and literature data.
- Chlorobenzene retardation factor (R) was calculated by MT3DMS from field-measured bulk density values and calibrated Kd values estimated by PEST. The allowable range was 1 to 90.

- Benzene Kd was fixed at values ranging from 0.002 to 0.32 ml/g, based on field data and literature values.
- Benzene retardation factor (R) was calculated by MT3DMS from field-measured bulk density values and Kd, and had a range from 1.01 to 6.5.
- Benzene half-life was allowed to range from 30 to 1,000,000 days, to encompass the potential range of conditions including very rapid decay and virtually no decay.
- Source concentrations were allowed to range from 0.001 to 500,000 micrograms per liter ($\mu g/L$) for chlorobenzene, from 0.001 to 1,800,000 $\mu g/L$ for benzene, and from 0.001 to 1,000,000 $\mu g/L$ for p-CBSA. The low limits of these ranges were designed to allow the flexibility to account for the relatively coarse grid compared to the potential size of the actual source (i.e., the model source could not be smaller than a single grid cell of 100 by 100 feet, which could be a substantial overestimation of the source size in certain instances and had to be corrected by reducing the source strength). The upper limits of these ranges represent the corresponding solubility limits of these constituents.
- Source start time was assumed to be 1945.

Preferred Values for Model Parameters

A "preferred condition" for each calibration parameter was defined by the regularization equations as a set of preferred parameter values, from which deviations are tolerated only to the extent that they are supported by the data. The preferred values for model calibration parameters and the rationale for these values are presented in Table 3-2.

TABLE 3-2
Preferred Values for Model Parameters

Parameter	Location	Preferred Value	Units	Rationale
Flow				
River Conductance	Dominguez Channel	5,500	ft ² /day	Channel geometry and previous investigations
Recharge		1	in./yr	Professional judgment based on local climate and surface characteristics
Specific Yield		0.01		Professional judgment based on pilot test analysis
Specific Storage		2x10 ⁻⁶	1/ft	Professional judgment based on pilot test analysis
Horizontal Hydraulic Conductivity	UBF	1.9	ft/day	Geometric mean of aquifer test data in this HSU
	MBFB	20	ft/day	Geometric mean of aquifer test data in this HSU
	MBFM	0.1	ft/day	Professional judgment based on previous calibration results
	MBFC	10 to 150	ft/day	Professional judgment based on previous calibration results

TABLE 3-2
Preferred Values for Model Parameters

Parameter	Location	Preferred Value	Units	Rationale
	LBF	0.0008 to 0.27	ft/day	Professional judgment based on previous calibration results
	Gage	16 to 120	ft/day	Professional judgment based on previous calibration results
	GLA	0.017	ft/day	Professional judgment based on previous calibration results
	Lynwood	113	ft/day	Geometric mean of aquifer test data in this HSU
In addition, the results of	f 132 short-term	aquifer tests fr	rom the RI	were used as preferred-value targets.
Horizontal/Vertical Hydraulic Conductivity Ratio	UBF	200		Professional judgment based on previous calibration results
	MBFB	5		Professional judgment based on previous calibration results
	All others (fixed)	10		Professional judgment based on hydrogeological literature
Transport				
Longitudinal dispersivity	All layers	10	Ft	Based on scale of chlorobenzene plume
Transverse to longitudinal dispersivity ratio	All layers	0.5		Professional judgment based on hydrogeological literature
Vertical to longitudinal dispersivity ratio	All layers	0.001		Professional judgment based on hydrogeological literature
Chlorobenzene source	MBFB	350,000	μg/L	Professional judgment based on field data
concentration	MBFM	350,000	μg/L	Professional judgment based on field data
	MBFC	15,000	μg/L	Professional judgment based on field data
	LBF	10,000	μg/L	Professional judgment based on field data
	Gage	7,000	μg/L	Professional judgment based on field data
Chlorobenzene Kd	UBF	0.0053	ml/gal.	Field samples and literature values
	MBFB	0.039	ml/gal.	Field samples and literature values
	MBFM	0.018	ml/gal.	Field samples and literature values
	MBFC	0.13	ml/gal.	Field samples and literature values
	LBF	0.43	ml/gal.	Field samples and literature values
	Gage	0.27	ml/gal.	Field samples and literature values
	GLA	0.73	ml/gal.	Field samples and literature values
	Lynwood	0.53	ml/gal.	Field samples and literature values

TABLE 3-2
Preferred Values for Model Parameters

Parameter	Location	Preferred Value	Units	Rationale
Benzene source concentration	UBF	3,000 to 1,200,000	μg/L	Professional judgment based on field data
	MBFB	3,100 to 1,200,000	μg/L	Professional judgment based on field data
	MBFM	3,000 to 275,000	μg/L	Professional judgment based on field data
	MBFC	60 to 190,000	μg/L	Professional judgment based on field data
Benzene half-life	UBF	84	Days	Professional judgment based on field data
	MBFB	84	Days	Professional judgment based on field data
	MBFM	84	Days	Professional judgment based on field data
	MBFC	84	Days	Professional judgment based on field data
	LBF	300	Days	Professional judgment based on field data
	Gage	300	Days	Professional judgment based on field data
	GLA	300	Days	Professional judgment based on field data
	Lynwood	300	Days	Professional judgment based on field data
p-CBSA source	MBFB	500,000	μg/L	Professional judgment based on field data
concentration	MBFM	500,000	μg/L	Professional judgment based on field data
	MBFC	450,000	μg/L	Professional judgment based on field data
	LBF	150,000	μg/L	Professional judgment based on field data
	Gage	50,000	μg/L	Professional judgment based on field data

ft/day – feet per day ft2/day – square feet per day

The Work Plan Amendment (CH2M HILL, 2006a) proposed a methodology to incorporate the statistical features of a large number of short-term aquifer tests as calibration targets. However, preliminary analysis of pilot testing results suggested that for the MBFC aquifer, the short-term aquifer tests performed during RI potentially overestimated hydraulic conductivity by a factor of two. The pilot testing data are of much higher quality, and therefore, short-term aquifer testing results were converted to regularization-type (i.e., lower weight) preferred-value targets. As lower-weight targets, these values influenced estimated properties only if other calibration targets did not provide much information about aquifer properties at those locations.

3.1.3 Calibration Targets

Five main groups of calibration targets were selected for calibration. These groups include (1) the 2006 baseline water level data (heads), (2) head differences calculated from the 2006

baseline water level data, (3) transient drawdown and buildup from eight extraction and four injection tests, (4) all available concentration data for chlorobenzene, benzene, and p-CBSA (i.e., data from 1983 through 2006), and (5) chlorobenzene and p-CBSA mass targets estimated based on kriging of concentration data. The calibration targets were subgrouped by model aquifer layers (1, 2, 4, 5, 9, and 13), for which these targets were available.

Calibration weights were developed empirically, and were adjusted during the calibration process to improve the match between the observed and simulated results. Calibration was focused on the most pertinent aspects with regard to the modeling objectives, such as aquifer test responses and the distribution of chlorobenzene concentrations that are above in situ groundwater standards (ISGS) in the MBFC and Gage aquifers. The groups of calibration targets and weighting of these targets in the calibration process are discussed below.

Heads

All 2006 baseline water level data collected by Shell and Montrose and available 2006 data collected by Boeing and TRC were used as calibration targets. In addition, available water level data collected near the Mobil site in a similar timeframe were considered. However, water levels collected near the Mobil site were given less weight, because of the uncertainty associated with the field procedures and timeframes for water level measurements, and because the screen intervals of Mobil wells were not always appropriate for incorporation into the model (i.e., many wells had long screens and were screened across multiple layers). All other water level measurements were initially assigned equal weights in the calibration process. In the process of calibration, the weights were increased for the selected water table wells in the vicinity of the Del Amo site to achieve a better overall match between the measured and simulated water levels.

Vertical Head Differences

Vertical head difference calibration targets were calculated for 70 locations where two or more wells screened in different HSUs were located within 20 feet of each other. This distance was selected because given an average lateral gradient of 0.001 foot per foot (ft/ft) in the model domain, the distance of 20 feet would result in a maximum error of only 0.02 foot in estimates of vertical head differences. This amount of error is negligible given the average head difference of 1.57 feet in the 70 well pairs. Head differences were weighted by the inverse of the absolute value of the head difference, to equalize the importance of small and large head differences.

Pilot Test Data

As discussed above, a comprehensive pilot testing program was implemented by Montrose to obtain data on the hydraulic properties of the aquifers and aquitards, and specific capacities of injection and extraction wells (H+A, 2008). The pilot test pumping and injection created large-scale stresses on the aquifer system, and allowed measurement of water level changes in response to pumping/injection (i.e., water level drawdowns and buildups) in a number of wells in multiple HSUs.

Sequential transient calibration runs were performed to calibrate the model to the results of these pilot and aquifer tests. A total of 3,692 drawdown and buildup measurements were

used as calibration targets. Collectively, these measurements were the most important calibration targets for the flow portion of the RD model, because they constrain estimates of the hydraulic properties of the aquifers and aquitards and significantly reduce the uncertainty pertaining to the hydraulic properties of the model.

Simulated drawdown (or buildup) from monitoring wells located within 290 feet (i.e., two diagonal model cells away or less) of the pumping well, in the same aquifer as the pumping well, was corrected to remove the effect of model cell size on simulated drawdown. This correction was required because the simulated drawdown in a pumping cell was averaged over the cell, and did not represent drawdown at any specific distance from the pumping well. Consequently, model estimates of drawdown in monitoring wells located close to the pumping well (i.e., in the same or in adjacent model cells) were impacted by this averaging. In order to address this issue, the amount of drawdown per foot of (log-scaled) distance from the center of the pumping cell was calculated using drawdown data from two adjacent model cells located along a line. These values of drawdown per foot of (log-scaled) distance were used to calculate drawdown at the monitoring well located within or near the pumping cell. With this calculation, the correct relationship between distance from the pumping well and drawdown was preserved when comparing measured and simulated data.

Drawdown and buildup measurements were initially weighted to give each aquifer test equal importance in the objective function. These weights were adjusted iteratively during calibration by applying zero weight to measurements that appeared to be erroneous or noise, by increasing the weight on late-time data and on monitoring wells located close to the tested well, and by increasing the weight on the data from aquifer tests, which did not calibrate as readily as others.

Chlorobenzene Concentrations

All available chlorobenzene concentrations (i.e., for years 1983 through 2006) were used as calibration targets. The weights of chlorobenzene concentration calibration targets were adjusted several times in the process of calibration to achieve a better match between the observed and simulated distributions. A linear weighting scheme was initially used, based on the success of a similar scheme in the Data Gap Analysis calibration effort (CH2M HILL, 2005). Anomalous data points were given a zero weight, such as where a long-term concentration trend was interrupted by a single dissimilar data point, after which the trend resumed. Calibration weights were increased in recently installed wells, particularly Gage aquifer monitoring wells that defined the southwestern and southeastern lobes of the chlorobenzene plume to compensate for the absence of historic data points for these wells. In addition, weights were increased for wells that defined important characteristics of the chlorobenzene plume, such as wells near the toe of the plume and in high-concentration areas.

Benzene Concentrations

All available benzene concentrations (i.e., for years 1985 through 2006) were used as calibration targets. The weights of benzene concentration calibration targets were adjusted several times in the process of calibration to achieve a better match between the observed and simulated distributions. A linear weighting scheme was initially used, based on the success of a similar scheme in the Data Gap Analysis calibration effort (CH2M HILL, 2005).

Anomalous data points were given a zero weight, such as where a long-term concentration trend was interrupted by a single dissimilar data point, after which the trend resumed.

Benzene concentrations within the chlorobenzene plume were given zero weight, because the origin of benzene within the chlorobenzene plume is uncertain. In addition, benzene in this area occurs at low concentrations, which will be treated as part of the chlorobenzeneplume remedy.

Weights were increased for nondetect values, in order to better reproduce the lateral and vertical extent of the benzene plumes. In addition, selected wells were given greater weight in order to correct deficiencies in the calibration and improve the overall match between measured and simulated results.

p-CBSA Concentrations

All available p-CBSA concentrations (i.e., for years 1990 through 2006) were used as calibration targets. Concentrations of p-CBSA were weighted similarly to those of chlorobenzene.

Mass Targets

Mass targets for chlorobenzene and p-CBSA were developed based on kriging of available concentration data for a given year (i.e., for years 1983 through 2006). All mass targets had equal weights.

3.2 Calibration Results

This section discusses the baseline calibration of the RD model including the results of flow and transport calibration, contribution to objective function, and calibrated distributions of model parameters. Appendix A contains a DVD with an electronic copy of the complete calibrated model. As discussed above, the calibrated baseline model was provided to all stakeholders on the CH2M HILL FTP site, discussed in detail at the modeling meetings and conference calls, and approved by Shell and Montrose as an appropriate tool for the wellfield optimization.

3.2.1 Flow Calibration

The results of the flow calibration are presented in Figures 3-1 through 3-3 and Figures 3-4A through 3-4D. Figure 3-1 presents a scatter diagram of simulated versus measured water levels (heads) and calibration statistics. Figure 3-2 presents simulated water level contours and water level contours interpreted from measured water levels for model layers 2, 5, and 9 representing the water table, MBFC, and Gage aquifers. Figure 3-3 presents simulated versus observed vertical head differences. Figures 3-4A through 3-4D present simulated drawdown contours and posted values of measured and simulated drawdown (or buildup) at the end of four extraction and four injection tests. These figures also show the residual drawdown/buildup, which is the difference between the observed and simulated values. Appendix B presents simulated and measured drawdown (or buildup) hydrographs from eight extraction and four injection tests that were simulated as part of the calibration process for a large number of observation wells and pumping and injection wells.

Figures 3-1 through 3-4D demonstrate a good agreement between the observed and simulated water levels, vertical head differences, and aquifer test drawdown/buildup. The scatter plot of measured and simulated water levels shown in Figure 3-1 has a slope that is similar to the line of perfect agreement (i.e., 1:1 slope), and is located relatively close to this line, indicating a good agreement between the simulated and measured heads in all units.

The calibration error, as measured by the root mean squared (RMS) of simulated heads versus measured water level elevations, is 0.66 foot when data for all 320 monitoring wells are considered; this also indicates a good match between observed and simulated water levels.

The comparison of interpreted and simulated water level contours in Figure 3-2 shows a close match. Spatial changes in flow directions and gradients indicated by field data are reproduced by the calibrated model.

The scatter plot of measured and simulated vertical head differences shown in Figure 3-3 is also located close to the line of perfect agreement, indicating good agreement between the simulated and measured vertical head differences. The use of vertical head differences between the model layers as calibration targets allowed better estimates of vertical hydraulic conductivities than using water levels alone.

The maximum drawdown and buildup plots shown in Figures 3-4A through 3-4D demonstrate a good match between measured and simulated response to groundwater extraction and injection. The hydrographs in Appendix B also demonstrate that a good match between simulated and measured aquifer response is achieved at both small and large distances from the tested well, across aquifer units, and at both early and late times in the simulation.

3.2.2 Transport Calibration

The results of transport calibration are presented in Figures 3-5 through 3-7 for chlorobenzene, benzene, and p-CBSA. Appendix C contains chemographs for hundreds of monitoring wells comparing simulated and measured chlorobenzene, benzene, and p-CBSA concentrations. These results indicate a good match between measured and simulated concentrations of all three constituents. The model reproduces the observed difference in the orientation of the chlorobenzene and p-CBSA plumes in the MBFC and the Gage aquifers. The simulated chlorobenzene and p-CBSA plumes in the Gage aquifer are oriented slightly more to the east compared to the plumes of these constituents in the MBFC, which is consistent with field data. The model also reproduced the major features of the plume including the plume width, length, direction, and concentration gradient between the core and edge of the plume. The two lobes of the chlorobenzene and p-CBSA plumes identified in the Gage were reproduced by the model. This was achieved by reproducing the vertical migration of these constituents from the MBFC to the Gage aquifer, which is consistent with the conceptual interpretation of field data.

Simulated benzene concentrations also have a good match with the benzene field sampling data. The simulated distance between the high-concentration benzene sources and the $1-\mu g/L$ contour matches well with the interpreted field data. The areas where a good match between the simulated and measured data has not been achieved usually have sparse field measurements (e.g. in the MBFC aquifer, between monitoring wells SWL0065 and

SWL0018, where interpreted concentration contours have been extended from a monitoring well with a high detectable concentration to a distant monitoring well with concentrations at or near the detection limit).

3.2.3 Contribution to Objective Function

The contribution to the objective function from different calibration targets is presented in Figure 3-8. Calibration weights were designed such that the pilot test responses were the most important target group, with secondary contributions from water levels, chlorobenzene, benzene, and p-CBSA concentrations, and with vertical water-level differences and mass targets as tertiary targets. As a result, the baseline calibration accounts for a variety of measured and estimated parameters and is considered to be a reasonable representation of flow and contaminant transport conditions beneath the Dual Site.

3.2.4 Calibrated Distributions of Model Parameters

The calibrated distribution of horizontal and vertical hydraulic conductivity is presented in Figures 3-9A through 3-9H, and Figure 3-10. Note that for the HSUs represented by multiple model layers such as MBFC, LBF, and GLA, the distribution of these properties is the same in all layers representing a given unit, and only the top layer is shown on the figures. The calibrated recharge distribution is shown in Figure 3-11. Calibrated storage coefficients are presented in Table 3-3.

Calibrated transport parameters including porosity; longitudinal, transverse, and vertical dispersivity (D_L , D_T , and D_Z); Kd; R; bulk density; and chlorobenzene and p-CBSA source concentrations are presented in Table 3-4.

The values and distribution of model parameters obtained as a result of the baseline calibration are reasonable for the hydrogeologic system beneath the Dual Site. However, as discussed above, this combination of model parameters resulting in a good match between the observed and simulated conditions may not be unique, and may be one of many possible and equally reasonable combinations that could be obtained using PEST calibration. Consequently, as discussed in the failure analysis (Section 5 of this report), other combinations of model parameters were considered to assess the range of possible calibration solutions and the impact of these solutions on model predictions (see Section 5).

TABLE 3-3
Calibrated Storage Coefficients

	Parameter/	Well	Name										
HSU	Units	BF-22	BF-27	BF-28	BF-EW-1	BF-EW-2	BF-IW-1	BF-IW-2	G-EW-1	G-EW-2	G-EW-3	G-IW-1	G-IW-2
UBF	Sy	0.0044	0.095	0.029	0.035	0.013	0.065	0.0083	0.007	0.015	0.057	0.0095	0.0066
MBFB	Ss (1/ft)	2.3E-05											
MBFM	Ss (1/ft)	3.9E-05											
MBFC	Ss (1/ft)	1.9E-05	1.2E-06	1.3E-05	2.2E-06	2.1E-05	1.5E-06	3.4E-07	2.9E-07	2.9E-07	2.9E-07	2.9E-07	2.9E-07
LBF	Ss (1/ft)	3.2E-06											
Gage	Ss (1/ft)	1.3E-06	1.3E-06	1.3E-06	1.9E-07	1.9E-07	1.9E-07	1.9E-07	4.9E-06	4.9E-06	3.9E-06	4.1E-06	4.0E-06
GLA	Ss (1/ft)	9.8E-08											
Lynwood	Ss (1/ft)	1.7E-07											

Notes:

Sy – Specific yield

Ss – Specific storage

TABLE 3-4
Calibrated Transport Parameters

HSU	Porosity	D _L (ft)	D _T (ft)	D _z (ft)	Chlorobenzene Source (µg/L)	Chlorobenzene Kd (ml/g)	Chlorobenzene R (n _{eff} = n)	p-CBSA Source (µg/L)	Benzene Kd (ml/g)	Benzene R (n _{eff} = n)	Benzene Half-Life (days)	Bulk Density (g/cm³)
UBF	0.20	32	0.5	0.00100		0.0052	1.04		0.002	1.01	83	1.49
MBFB	0.20	2.8	0.39	0.00088	310,000	0.069	1.51	490,000	0.012	1.09	130	1.49
MBFM	0.12	2.4	0.49	0.00044	310,000	0.018	1.19	490,000	0.0062	1.06	84	1.25
MBFC	0.12	63	0.5	0.00025	23,000	0.023	1.30	160,000	0.042	1.56	84	1.59
LBF	0.05	44	0.5	0.00048	16,000	0.1	4.04	120,000	0.18	6.47	300	1.52
Gage	0.12	15	0.19	0.00100	11,000	0.045	1.57	51,000	0.11	2.40	300	1.53
GLA	0.12	24	0.5	0.00099		0.72	10.06		0.28	4.52	300	1.51
Lynwood	0.12	31	0.5	0.00100		0.052	1.76		0.32	5.69	300	1.76

Notes:

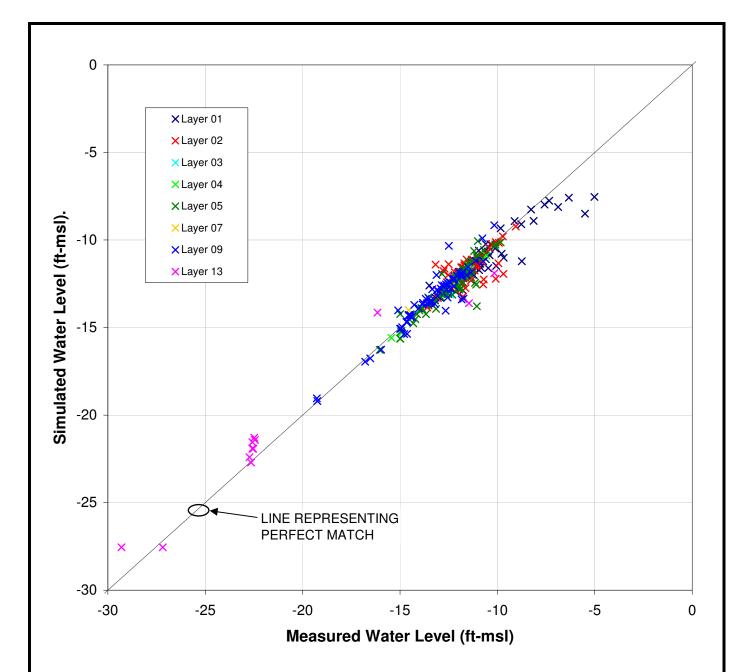
g/cm³ – grams per cubic centimeter

 $D_L-longitudinal\ dispersivity$

 $D_{T}-transverse \ to \ longitudinal \ dispersivity$

Dz - vertical to longitudinal dispersivity

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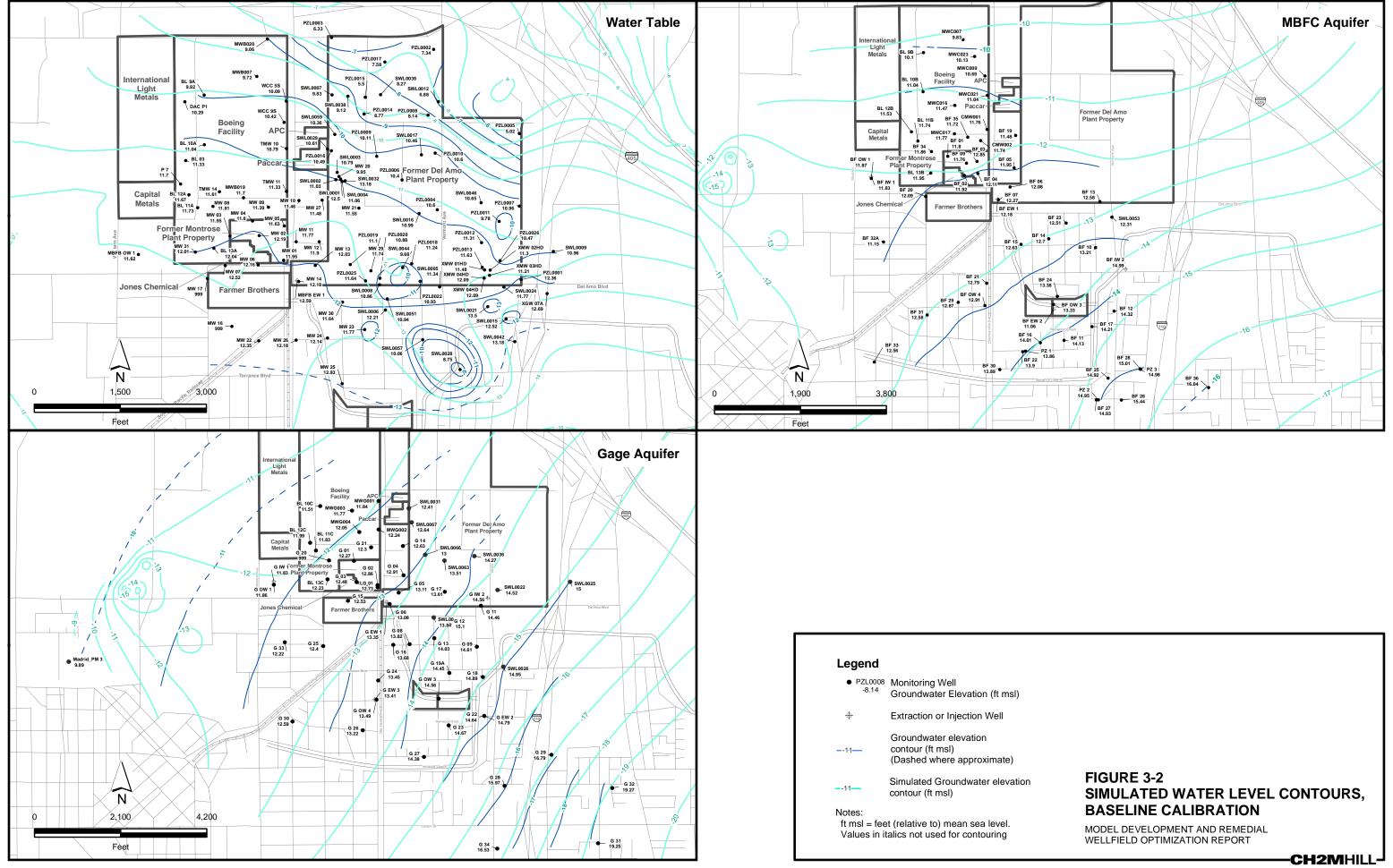


Water Level Residual Statistics

=0.000 0	
Count	320
Measured Maximum	-5.02 ft-msl
Measured Minimum	-29.30 ft-msl
Measured Range	24.28 ft
Maximum Residual	2.99 ft
Minimum Residual	-2.17 ft
Mean Residual	0.21 ft
Absolute Mean Residual	0.44 ft
Root Mean Squared Residual	0.66 ft
RMS/Range	2.7%

FIGURE 3-1 SIMULATED VS. MEASURED WATER LEVELS, BASELINE CALIBRATION

MODEL DEVELOPMENT AND REMEDIAL WELLFIELD OPTIMIZATION REPORT



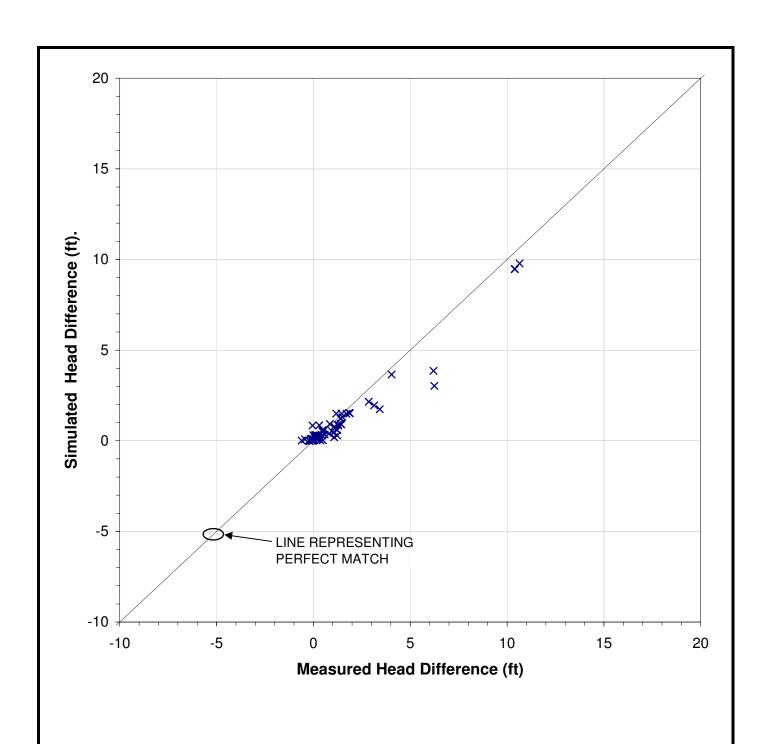
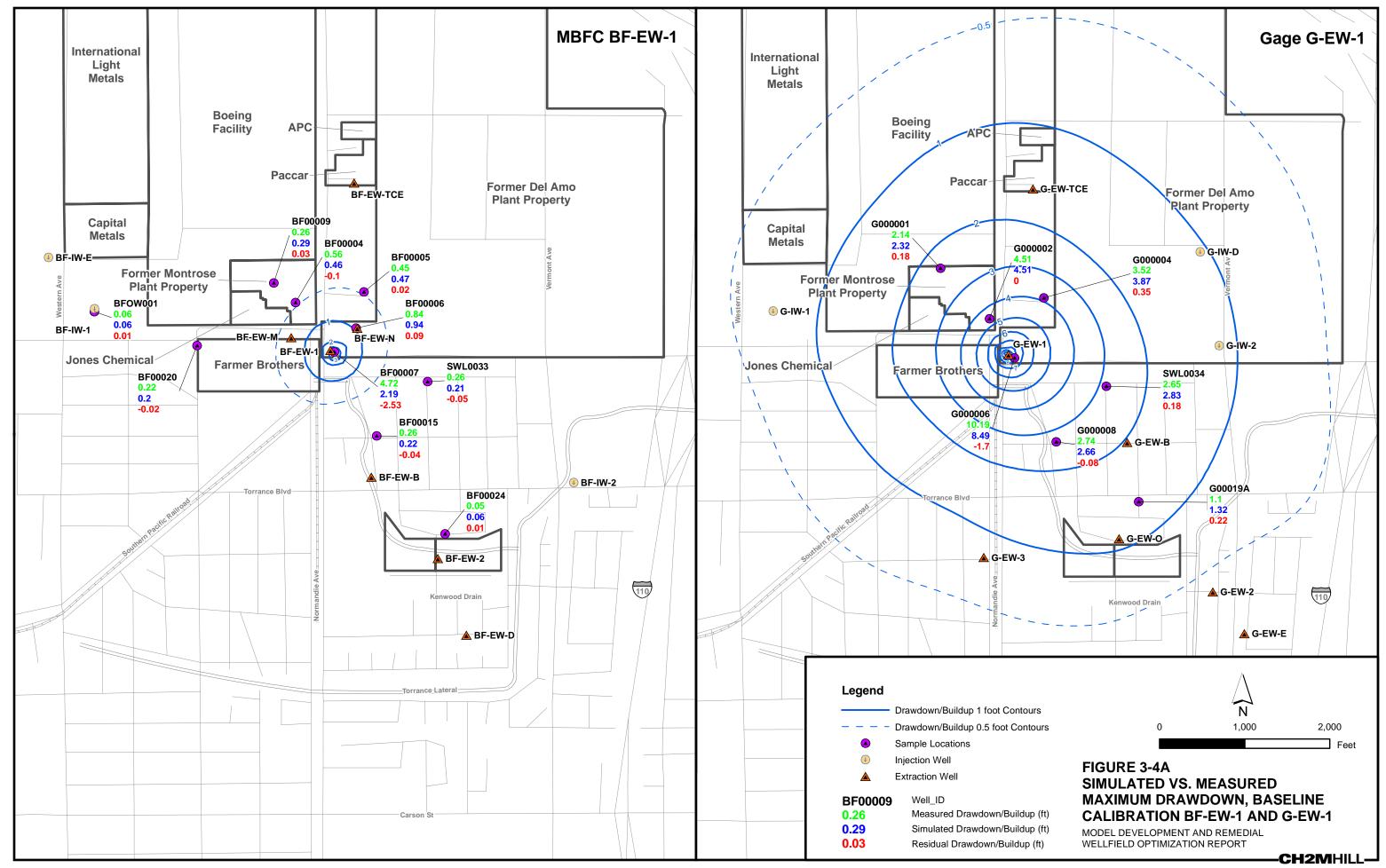
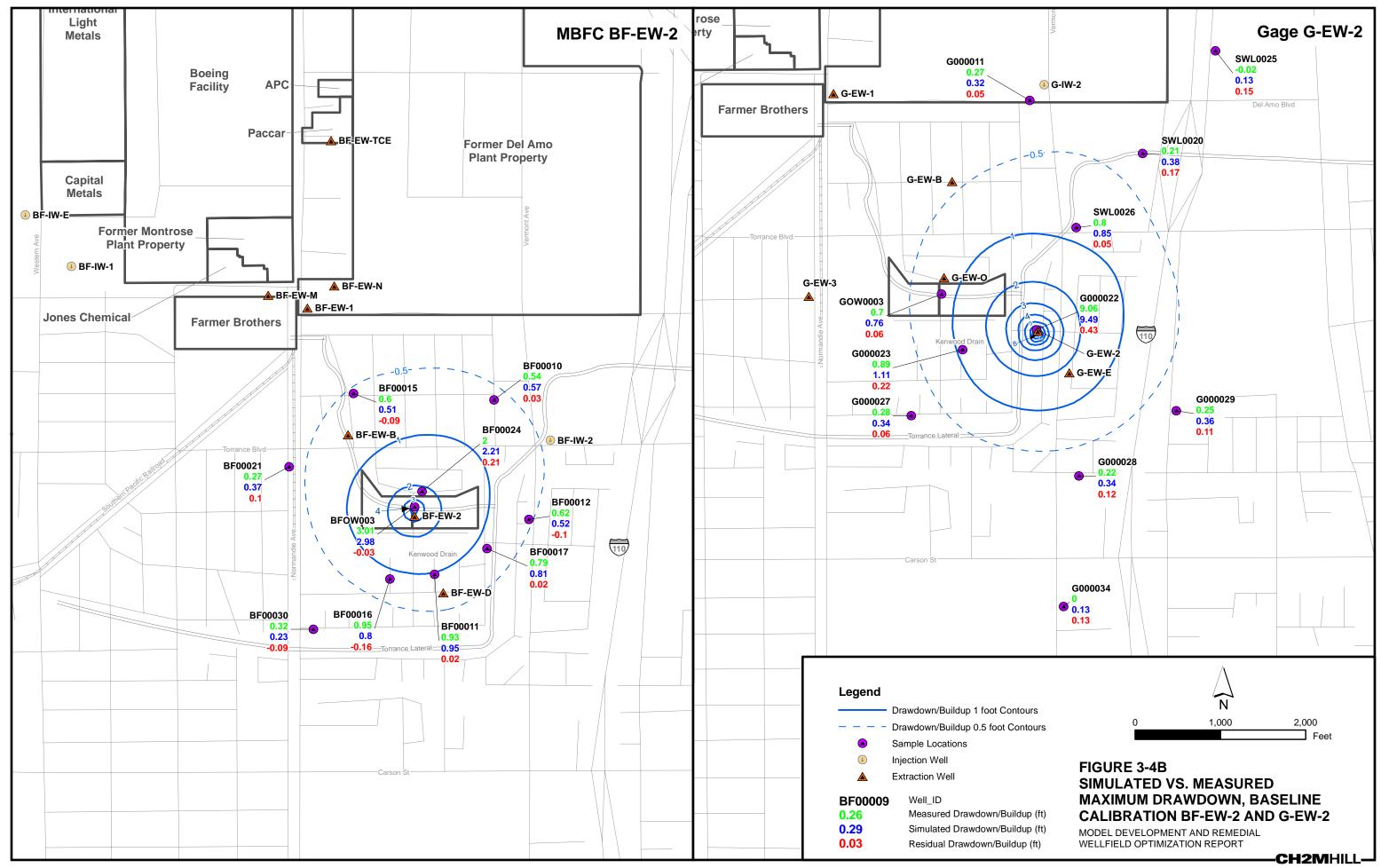
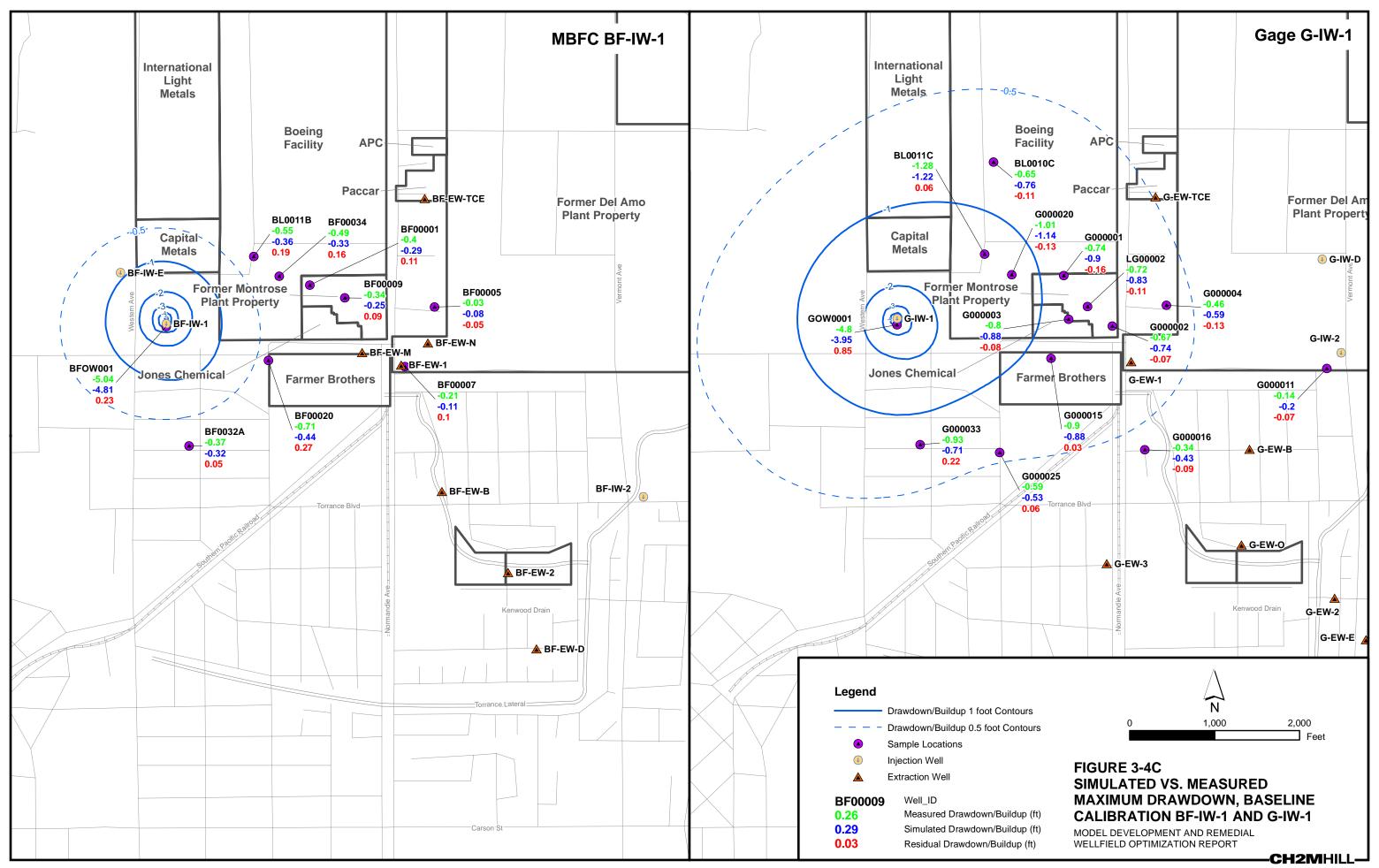


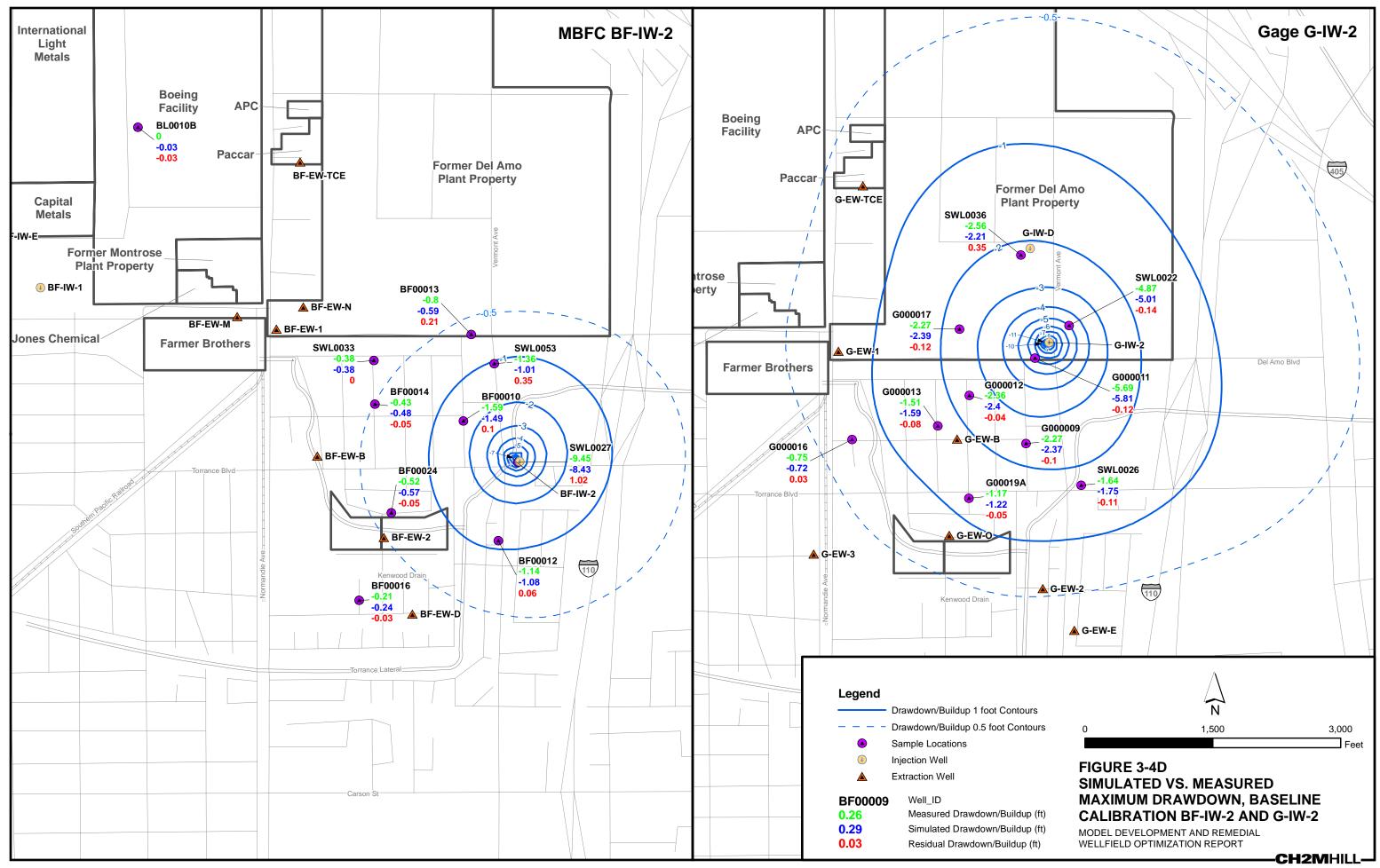
FIGURE 3-3
SIMULATED VS. MEASURED VERTICAL HEAD
DIFFERENCES, BASELINE CALIBRATION
MODEL DEVELOPMENT AND REMEDIAL

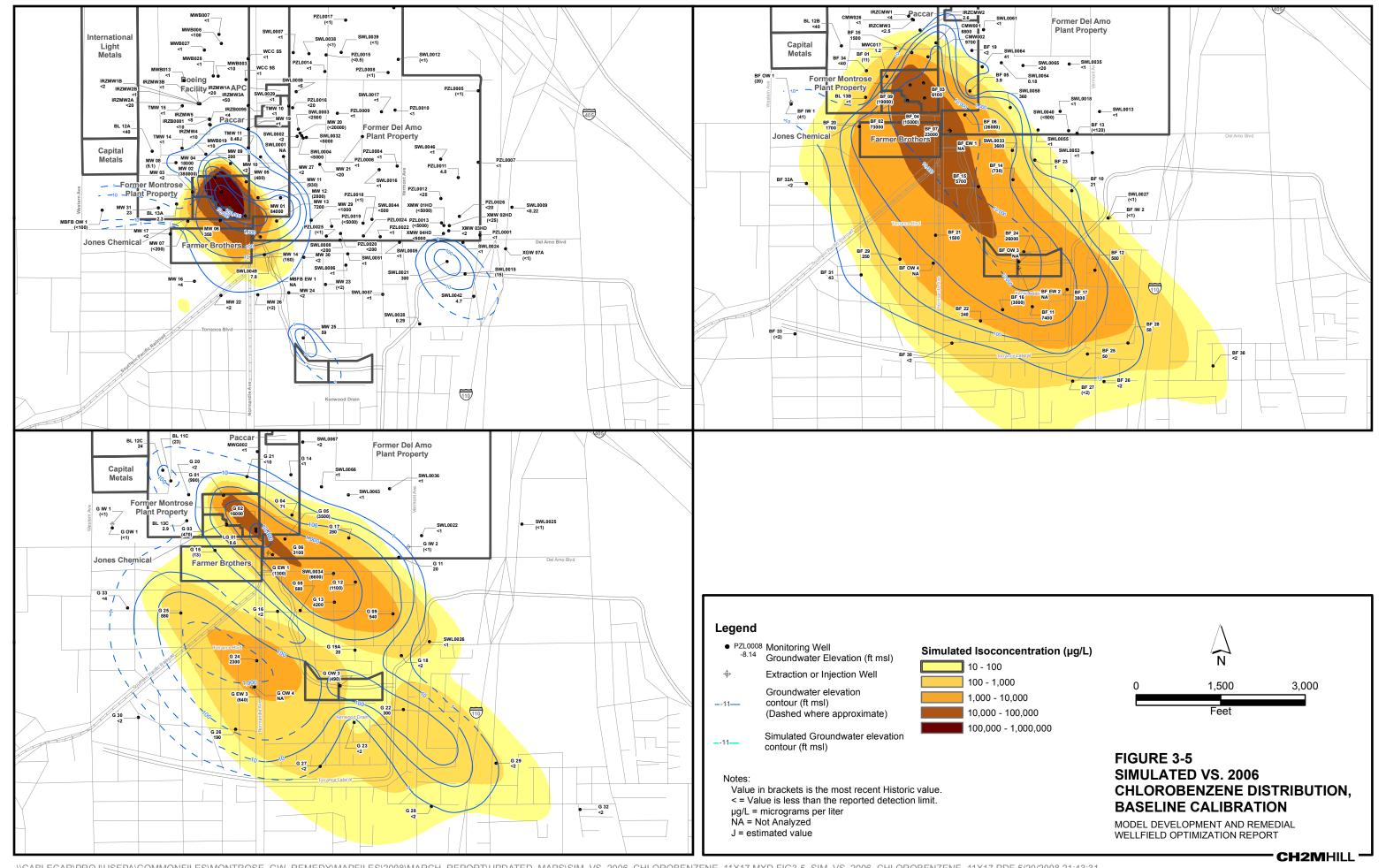
MODEL DEVELOPMENT AND REMEDIAL WELLFIELD OPTIMIZATION REPORT

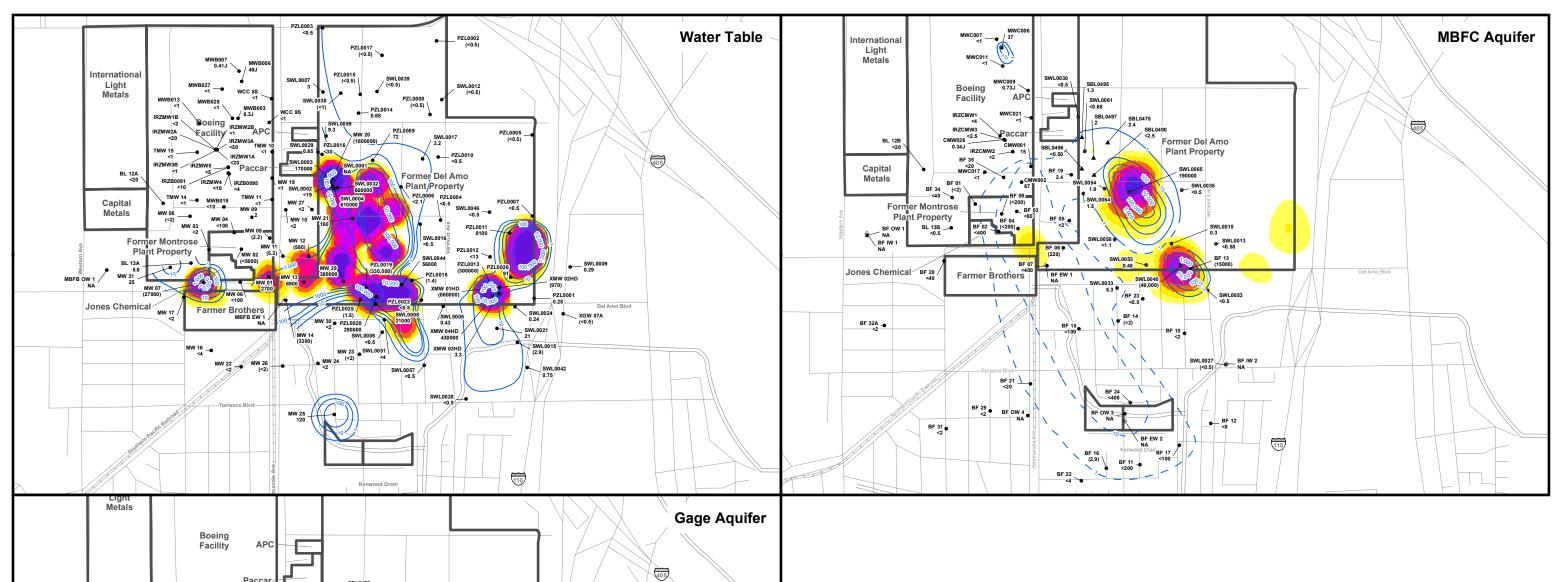


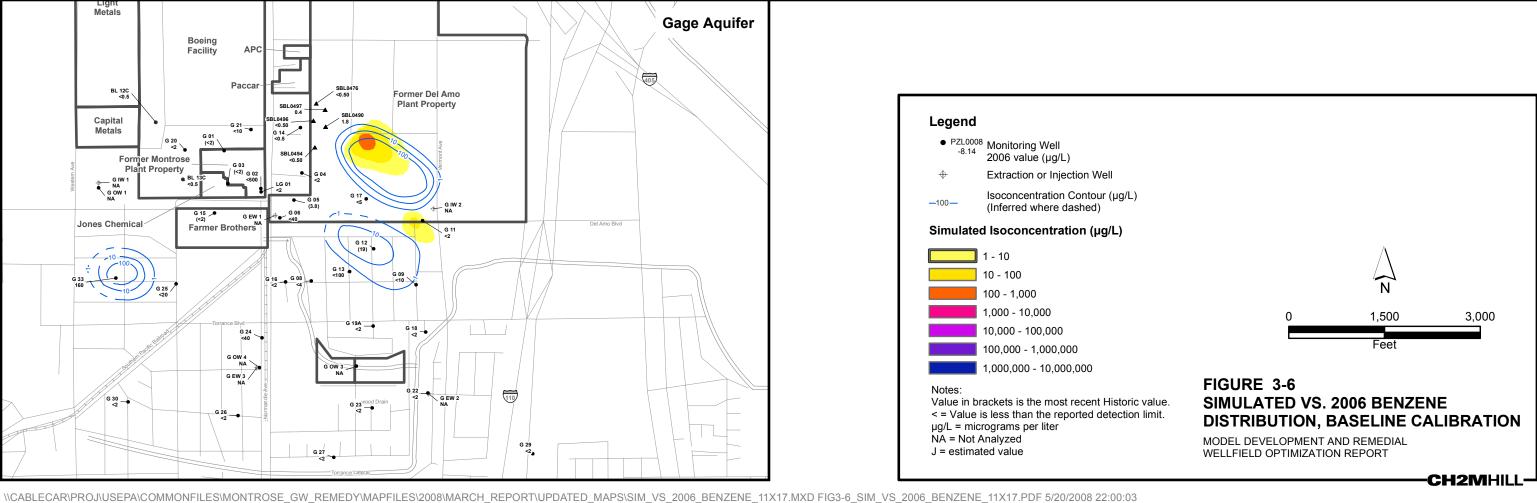


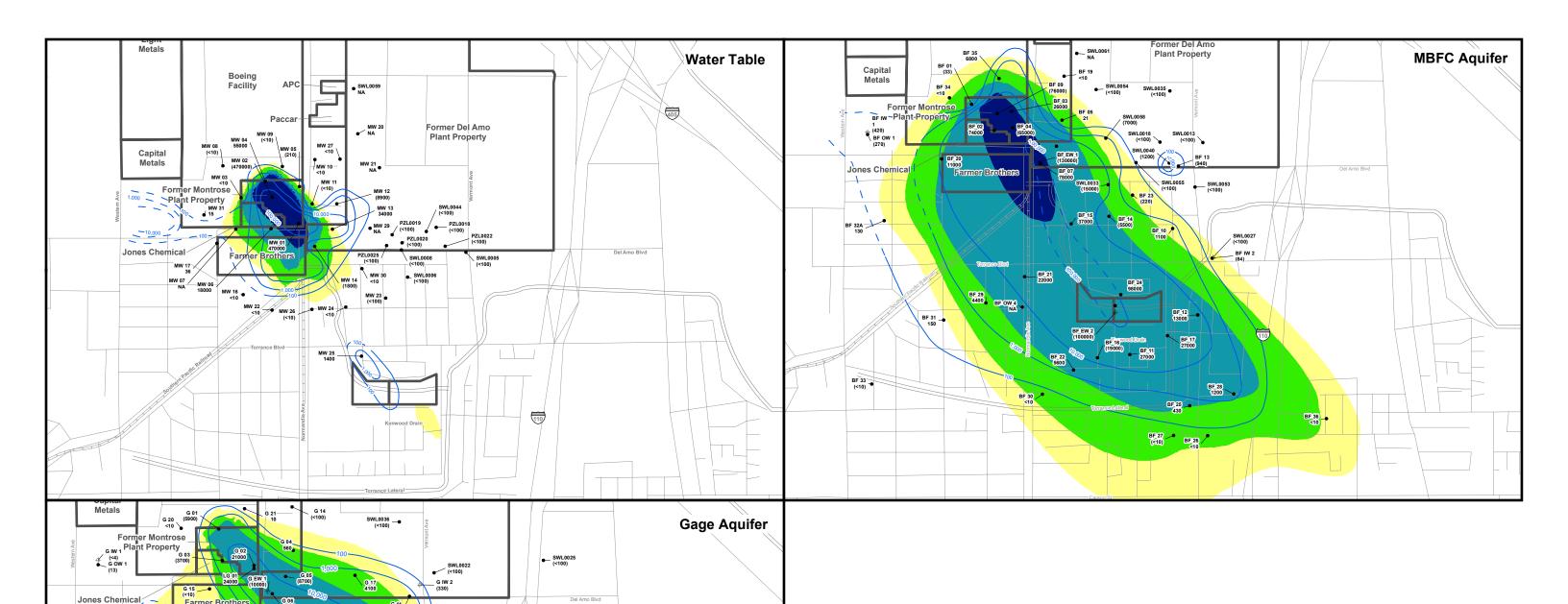


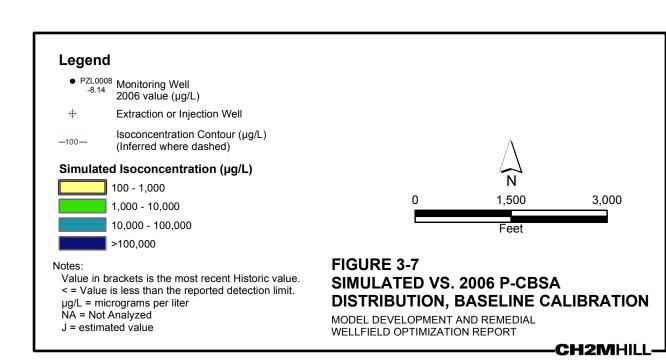




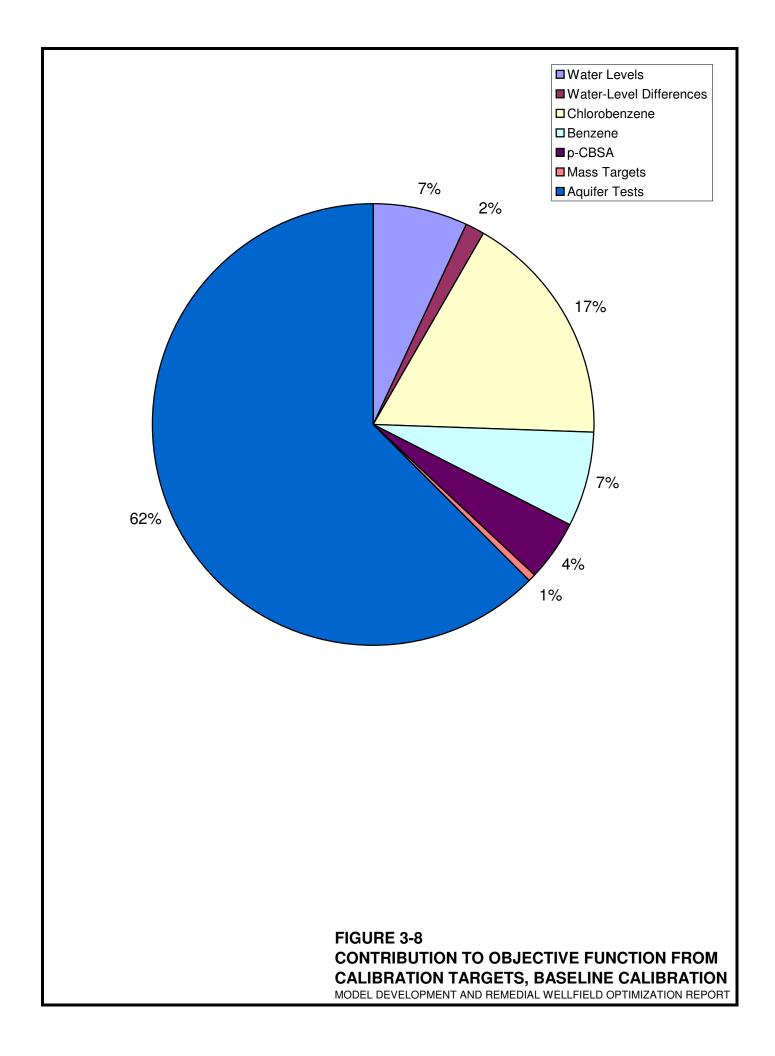


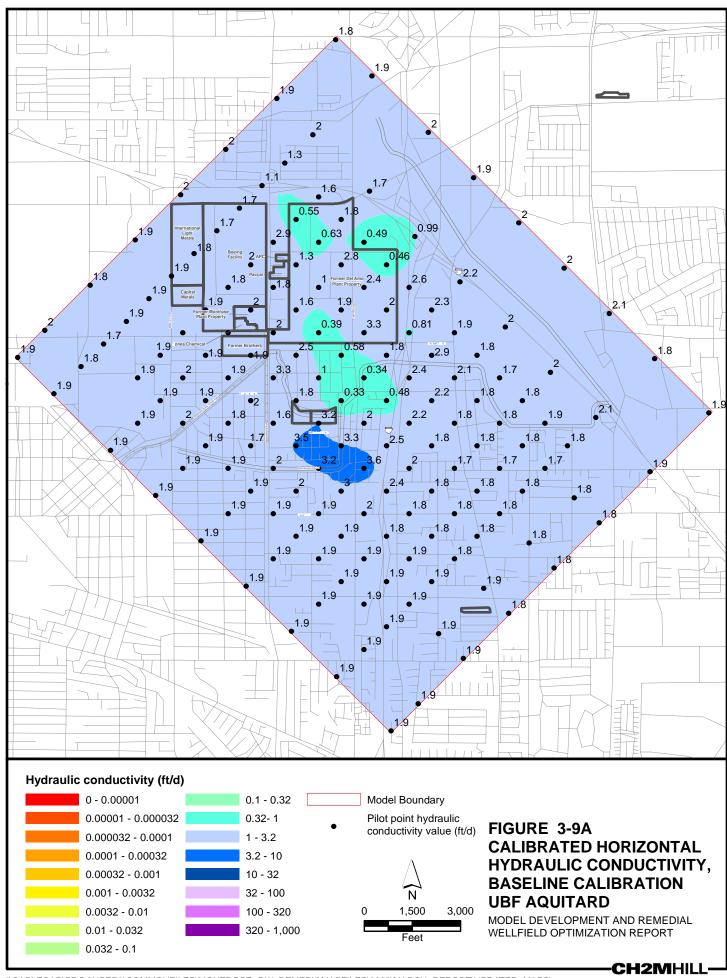


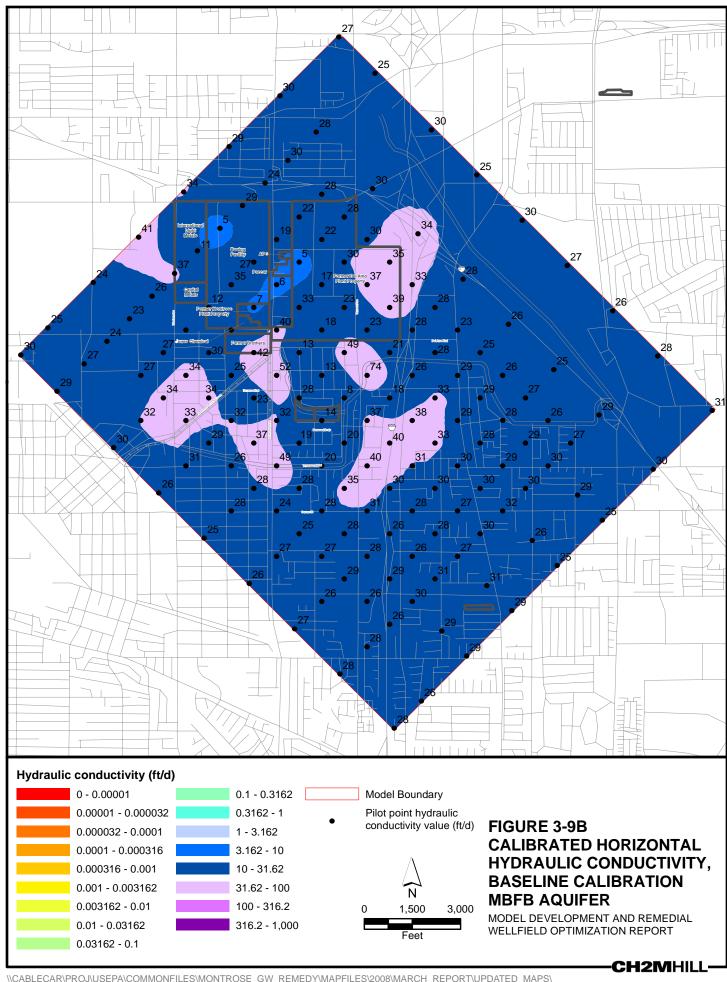


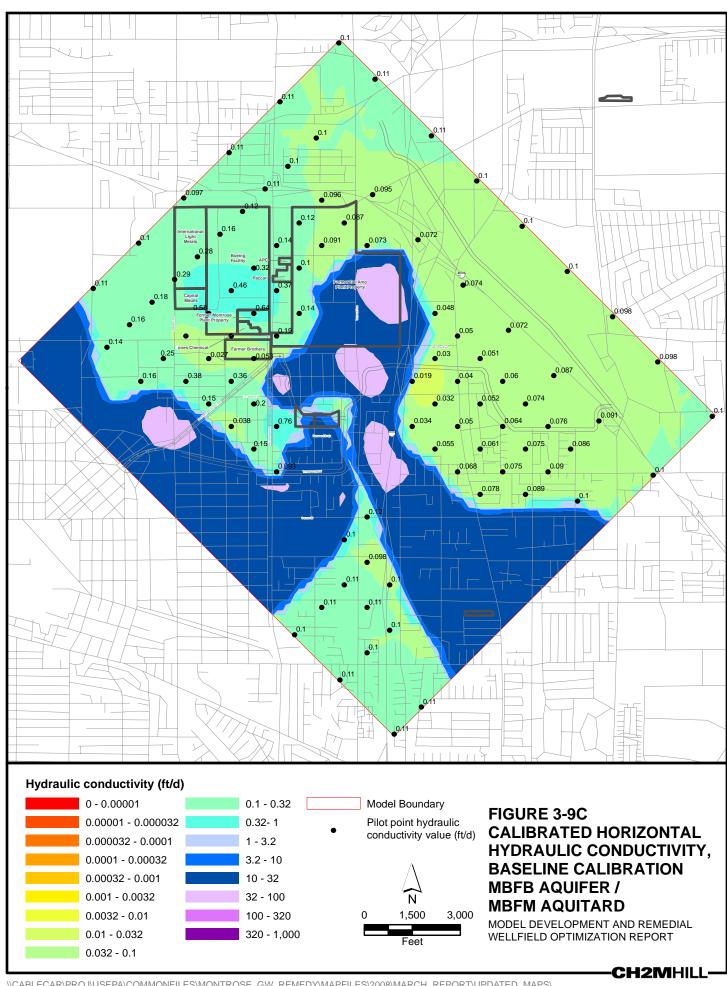


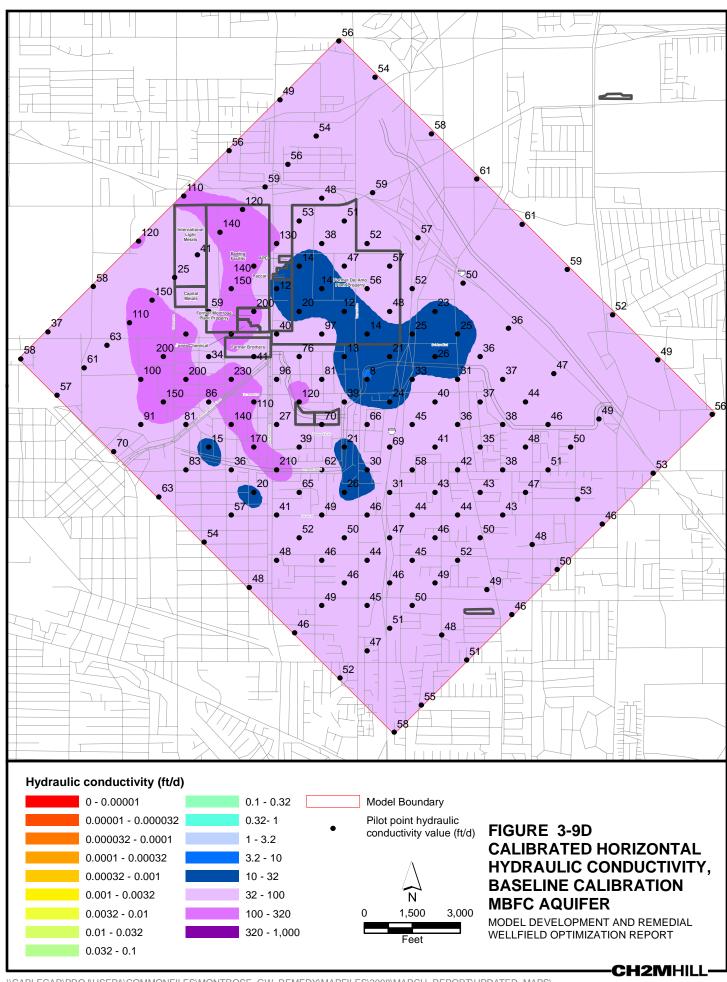
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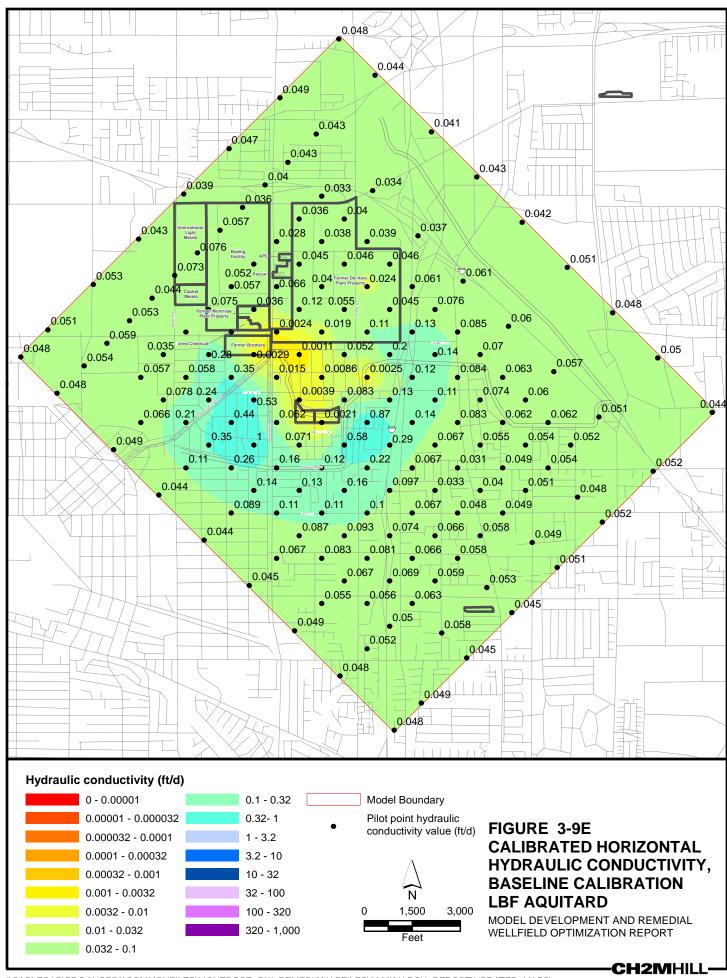


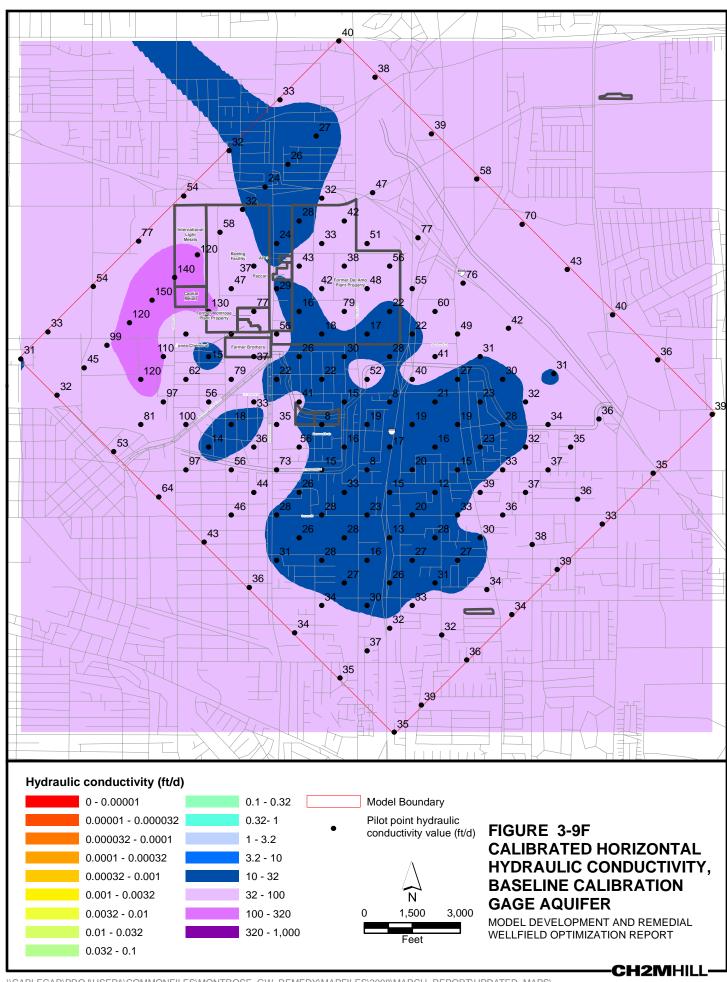


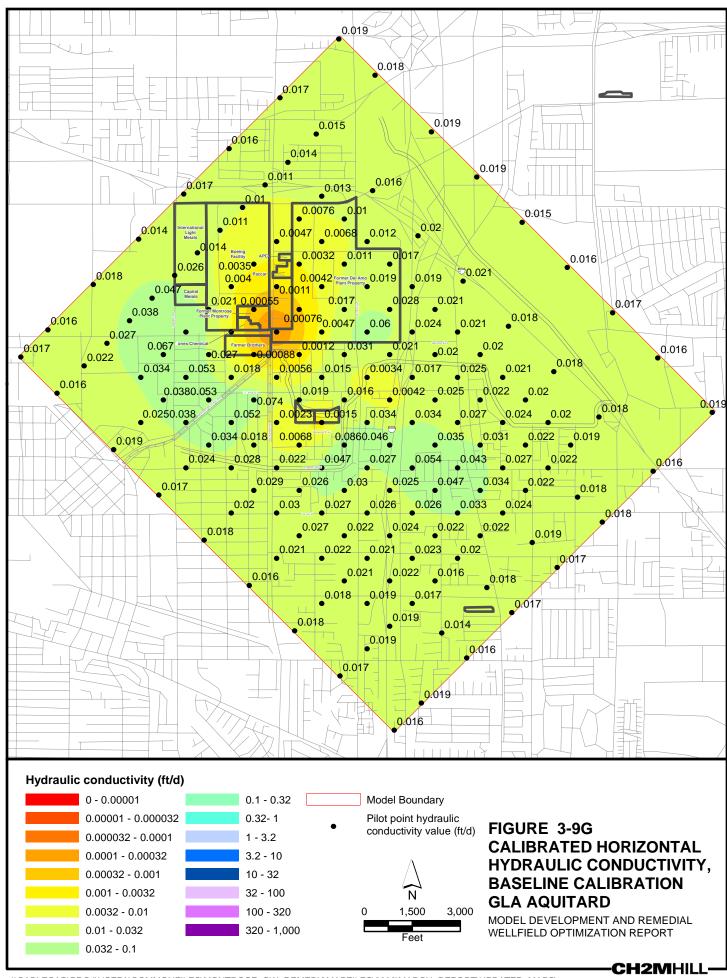


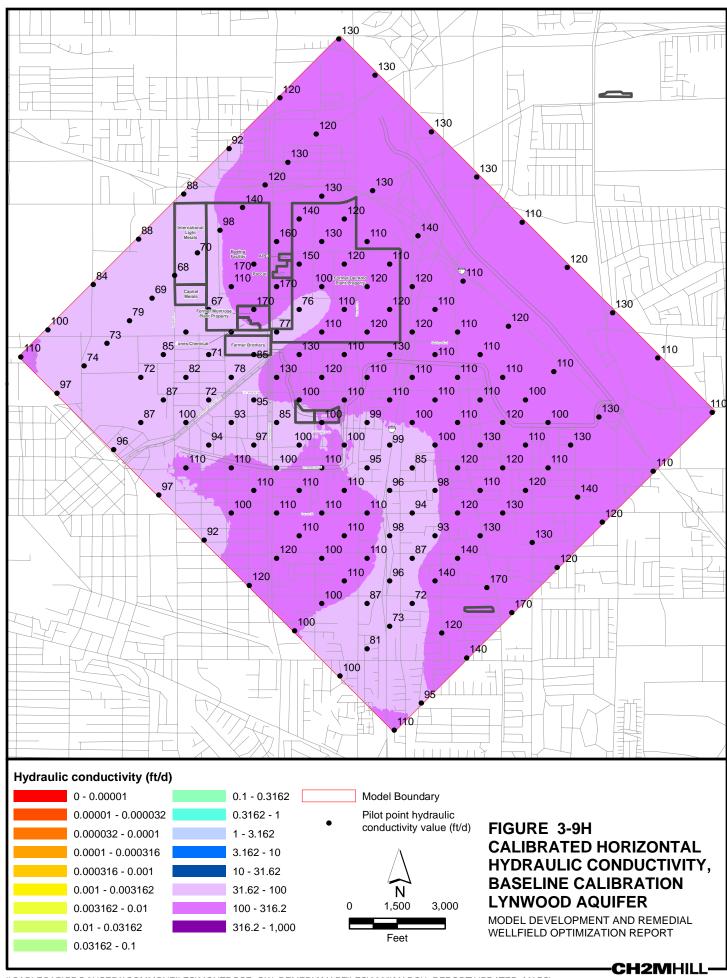


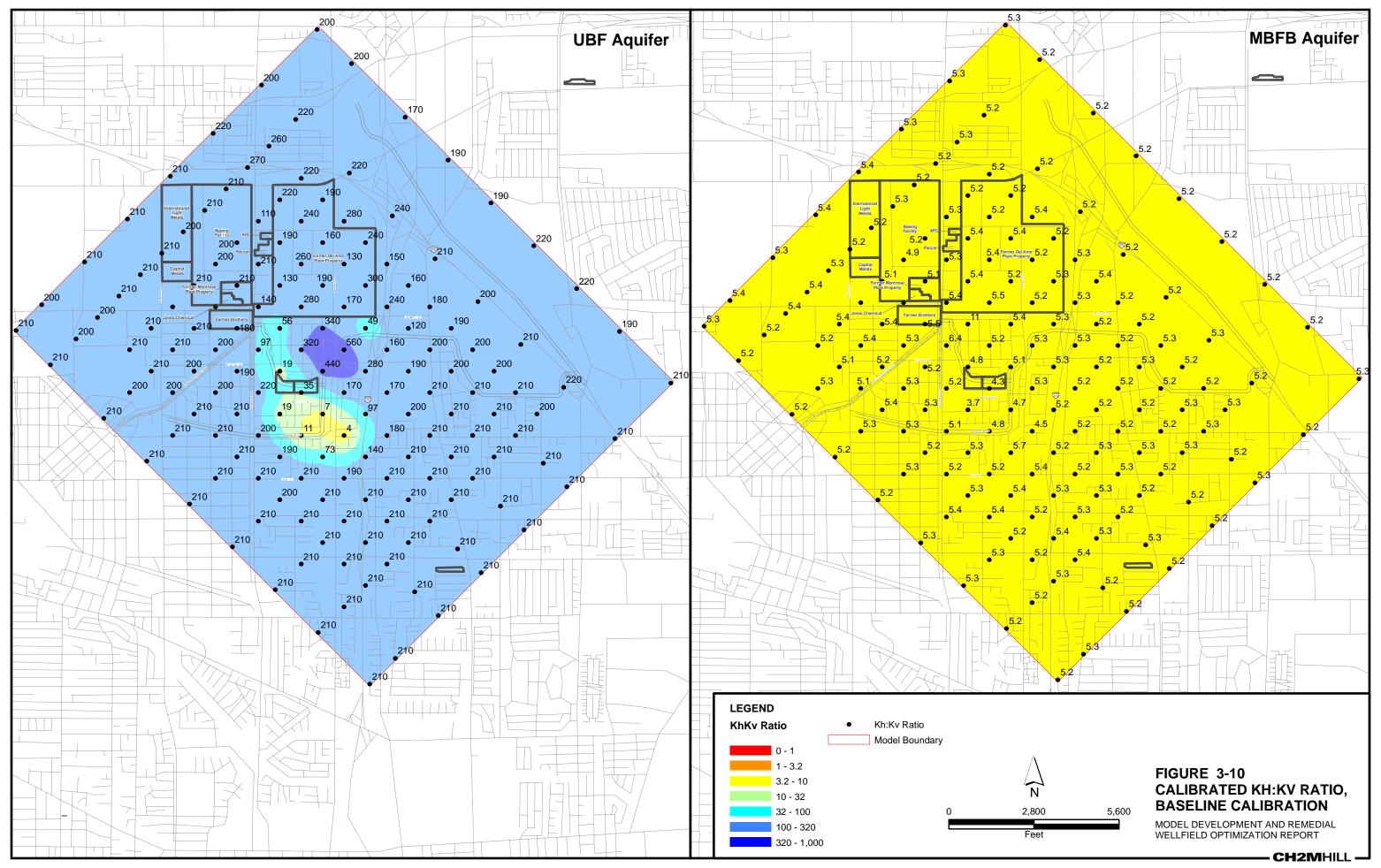


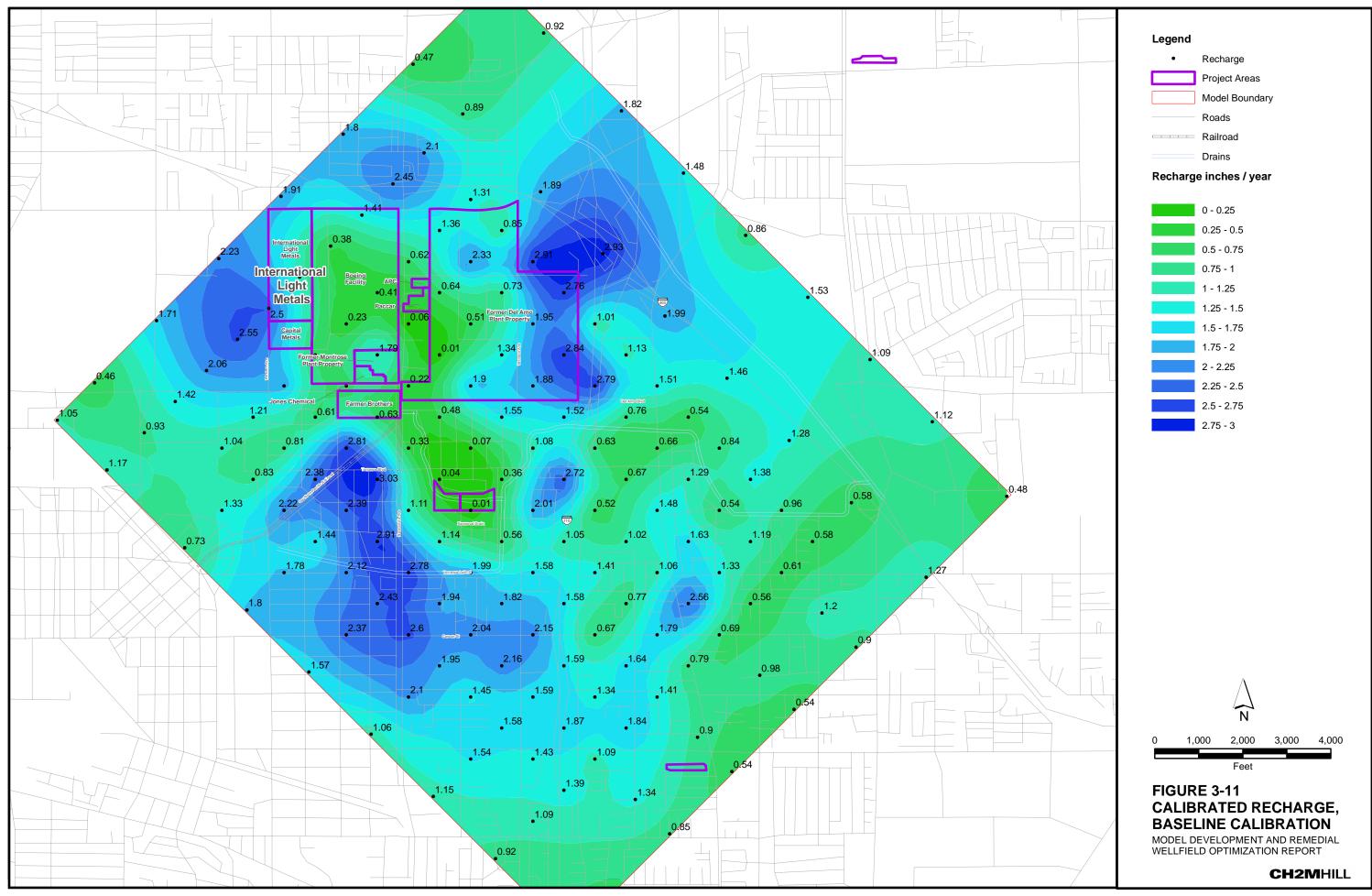












4. Wellfield Optimization

A calibrated RD model was used for the development and optimization of the remedial wellfield. The wellfield optimization methodology and the optimization results are discussed in this section.

4.1 Wellfield Optimization Methodology

The remedial wellfield optimization methodology described in this section was focused on the development of a remedial wellfield that can achieve all ROD requirements and account for design constraints in the most cost-effective manner. Specifically, the optimization process was used to determine the minimum pumping rate of the overall remedial wellfield that will meet these requirements within the design constraints. The overall pumping rate of the remedial wellfield is referred to as the "optimization target" in this analysis.

As discussed in Section 1 of this report, the ROD (EPA, 1999) mandates a number of design requirements and specifications for the remedial wellfield. Some of these requirements — including the minimum total pumping rate of the remedial wellfield, indefinite containment within the CZ, containment of the overall contaminant distribution, reduction of the volume of water with concentrations of contaminants above drinking water standards to zero within certain timeframes, and certain pore-volume flushing rates within the contaminant distribution—must be achieved by the remedial wellfield. These requirements are referred to as "hard remediation targets" for the purposes of this analysis.

Some other ROD requirements—including limiting adverse migration of contaminants and redistribution of groundwater extraction as the contaminant plume shrinks—should only be achieved to the extent that they do not interfere with the hard remediation targets. These requirements are referred to as "soft remediation targets." In addition, the wellfield design must account for constraints such as the access restrictions for the locations of wells and capacities of individual extraction and injection wells.

To summarize, the RD optimization process had to account for multiple remediation targets, some of which were more critical than others, and consider numerous design constraints. In addition, the optimization process had to account for the complicated conditions at the Dual Site, which included multiple contaminant plumes and source areas in multiple HSUs such as interconnected aquifers and aquitards. In order to account for this level of complexity, it was decided that automatic optimization would be performed using an optimization software package that would be linked to the RD model of the Dual Site.

Evaluation of several optimization software packages indicated that utilizing the optimization capabilities of PEST would be the most cost-effective approach for the remedial wellfield optimization. While optimization programs other than PEST could potentially also be used for the wellfield optimization, linking them to the RD model would be a difficult, time-consuming, and expensive task given the complexity of the model. In addition, other available optimization packages, such as global optimizer "Brute Force" or "Covariance

Matrix Adoption," would require a much longer run-time for the optimization runs. PEST, however, was already linked to the RD model as part of the calibration effort. In addition, the applicability and effectiveness of using PEST for the RD modeling has already been tested and confirmed during the previous stages of work, while the applicability and effectiveness of other optimization programs has not been tested, and further verification and confirmation would be required.

The mathematical procedure for PEST optimization is similar to that for calibration in terms of automatic minimization of the objective function. However, in the case of optimization, the objective function is the sum of squared residuals of the remediation targets, which include the ROD requirements, and the minimum flow rate optimization target.

In order to perform an automatic optimization using PEST, all ROD requirements as well as design constraints were translated into numerical measures that could be calculated at the end of a model run. The hard targets were given higher weighting than the soft targets. The pumping rate minimization target was set up as a "soft" target (i.e., a target that is preferred but not required), and had lower weighting than the remediation targets (i.e., ROD requirements). The optimization process was focused on minimizing the objective function by identifying the optimization parameters such as extraction and injection rates in individual remedial wells that were required to meet both the remediation targets and the overall pumping rate minimization target.

Because the ROD also requires that the remedial wellfield meet the remediation targets with a sufficient degree of certainty even if actual site conditions differ from those assumed by modeling, the optimization process was designed to ensure that the optimized wellfield performs well under a range of plausible conditions. This was achieved through failure analyses, which are discussed in detail in Section 5 of this report. The methodology for failure analyses is also discussed in the Initial Calibration and Data Gap Analysis Report (CH2M HILL, 2005).

The optimization approach discussed above allowed the development of a wellfield that is both reliable, with regard to achieving the remediation targets, and efficient, in that it uses the minimum amount of resources necessary to meet all remedial requirements. The remediation targets, design constraints, and the optimization target are discussed in detail below.

4.1.1 Remediation Targets

Establishing the quantitative procedure for the evaluation of the remedial wellfield performance with regard to meeting the ROD requirements was an important part of the optimization methodology development. To achieve this objective, the ROD requirements and specifications were translated into numerical targets that can be estimated by the model at the end of each optimization run. Specifically, the following remediation targets (or target groups) were developed based on the ROD requirements:

- Extraction rate target
- Plume capture targets
- Plume reduction and early time performance targets
- Limiting adverse migration targets

Some targets are evaluated on an annual basis, while others are evaluated for each stress period of the simulation (i.e., for each successive configuration of extraction and injection wells). The final weighting scheme for the remediation targets was developed iteratively, assigning greater weight to targets that were more difficult to achieve. A brief description of each target or target group is presented below.

Extraction Rate Target

Based on the ROD requirements, hydraulic extraction will be performed at a combined initial pumping rate (sum of pumping rates of all individual extraction wells) as close to 700 gpm as feasible. The pumping rate may be increased, if required, to meet other remediation targets. However, the pumping rate cannot be lower than 700 gpm. Consequently, the combined initial pumping rate of the remedial wellfield was not allowed to be less than 700 gpm in the PEST wellfield optimization simulations. However, the total extraction rate was allowed to decline from 700 gpm when extraction wells reached cleanup levels and were deactivated during the simulation.

Plume Capture Targets

Plume capture targets include capture inside the CZ and capture of the overall contaminant distribution. Each of these targets is discussed below.

Capture Inside the CZ

The ROD defines a CZ that was established on the basis of the technical impracticability (TI) waiver zone for the chlorobenzene and benzene plumes. The CZ surrounds the NAPL (both DNAPL and LNAPL) in the region of groundwater as defined in the ROD. The remedial actions should be implemented such that dissolved-phase contaminants and contaminants dissolving from NAPL within the CZ are prevented from escaping this zone and from entering the groundwater outside this zone (EPA, 1999). The remediation target for capture of the chlorobenzene plume inside the CZ was incorporated into the model using the particle-tracking code MODPATH (USGS, 1994), which allows the model to track the particles of groundwater migrating outside the CZ. Specifically, the following steps were implemented to incorporate the capture of the CZ target into the optimization simulations:

- One hundred particles were started on a horizontal plane halfway between the top and bottom of each model grid cell within the CZ, and tracked downstream to the location where they exited the model. Exit locations were defined as (1) remediation wells within the CZ, and (2) all other locations within the modeling domain.
- The number of particles captured within the CZ, and the number of particles that escaped the CZ were reported in the model output files for each stress period.

Capture inside the CZ was considered successful for each stress period if all particles exited the model at remediation wells inside the CZ. If any number of simulated particles of groundwater were escaping hydraulic extraction wells and migrating downgradient, the objective function was increasing above the desired value and the remedial wellfield was adjusted accordingly to improve the CZ containment.

Capture inside the CZ for the benzene plume could not be tracked using the particle-tracking routine. This is because particle tracking simulates advective transport (i.e.,

transport with groundwater flow), and does not account for other processes including biodegradation, which have significant impact on the benzene transport. Therefore, the CZ capture target for benzene was assessed using solute transport simulations. Specifically, a "newly contaminated area" target was incorporated into the optimization simulations. It was calculated based on the results of the solute transport simulations as the total area of model cells that exceed ISGS benzene levels for the current year, but not the previous year. This approach is discussed in detail in Section 4.1.1.5.

Capture of the Overall Contaminant Distribution

According to the ROD requirements, the site remedy shall achieve containment of the overall contaminant distribution, in a manner that does not permit the size of the chlorobenzene, benzene, and TCE plumes to increase once the remedial action is initiated. The chlorobenzene and benzene plumes were defined as the concentration distributions above the ISGS of these constituents including $70~\mu g/L$ for chlorobenzene and $1~\mu g/L$ for benzene. Because the distribution and sources of TCE were not as well characterized as those for chlorobenzene and benzene, a capture target for the TCE plume was defined as capture of all groundwater beneath the high-concentration source areas at the APC and PACCAR properties in the MBFC and Gage aquifers (see Section 2.8.4 and Figure 2-9). The capture target for the overall chlorobenzene distribution and for TCE distribution was incorporated into the model in a similar manner as the CZ capture target using the particle-tracking code MODPATH (USGS, 1994). Specifically, the following steps were implemented:

- One hundred particles were started outside the CZ within the chlorobenzene plume, and within the TCE plume at the APC and PACCAR properties. The particles originated on a horizontal plane halfway between the top and bottom of each model grid cell and were tracked downstream to the location where they exited the model. Particles were not started in model cells in the LBF and GLA aquitards, as the actual contaminant distribution in these units is highly uncertain. Exit locations were defined as (1) remediation wells, and (2) all other locations within the modeling domain.
- The number of particles captured within the CZ, and the number of particles that escaped the CZ were reported in the model output files for each stress period.

Capture of the overall contaminant distribution was considered successful for each stress period if all particles exited the model at remediation wells. If any number of simulated particles of groundwater were escaping hydraulic extraction wells and were migrating downgradient, the objective function was increasing above the desired value and the remedial wellfield was adjusted accordingly to improve the overall plume containment.

The target for capture of the overall distribution for benzene was estimated in the same manner as the CZ capture target for benzene, because the transport of benzene is impacted significantly by the process of biodegradation and cannot be assessed using particle tracking (see Section 4.1.1.2).

Plume Reduction and Early Time Performance Targets

Plume reduction and early time performance targets include plume reduction rates and pore-volume flushing rates. Each of these targets is discussed below.

Plume Reduction

As discussed in the ROD, it is an explicit objective of this remedy to achieve significant reduction in the volume of contaminated groundwater outside the CZ in the early time period as simulated by the EPA-approved RD model. To ensure that the remedy achieves the standards of the ROD in a reasonable timeframe, the ROD specifies volume-reduction rates for the chlorobenzene plume, with the focus on the MBFC and Gage aquifers (i.e., the main aquifers affected by the chlorobenzene contamination). It requires that, at a minimum, the rate of plume reduction achieves the following performance criteria when simulated by the EPA-approved RD model:

- 33 percent of the volume of the chlorobenzene plume outside the CZ shall be removed in 10 years.
- 66 percent of the volume of the chlorobenzene plume outside the CZ shall be removed in 25 years.
- 99 percent of the volume of the chlorobenzene plume outside the CZ shall be removed in 50 years.

Incorporation of the plume volume-reduction criteria into the model was accomplished as follows:

- It was assumed that because model layer thicknesses were relatively uniform within an HSU, it was acceptable to evaluate the percent reduction of the area of the plume as a proxy for volume.
- The plume area was estimated as the area of all model cells in the MBFC and Gage aquifers that were located within the chlorobenzene plume (i.e., within the distribution of chlorobenzene in groundwater that exceeds the ISGS level of 70 μ g/L), except for the area of the plume located inside the CZ.
- The plume-reduction calculations were further adjusted to ignore the area upgradient of the CZ, where the artificial propagation of the dissolved plume occurred as the result of numerical dispersion. Specifically, simulated chlorobenzene behavior near chlorobenzene source cells in the model showed some unrealistic effects, which were attributed to numerical dispersion. These artificial effects of numerical dispersion are not uncommon in MT3DMS solute transport simulations, and are a known shortcoming of the upstream finite-difference mathematical solution used by MT3DMS. Numerical dispersion resulted in upgradient propagation of concentrations in the MBFC aquifer (due to the particular combination of simulated flow conditions and transport properties in that area), which is not expected during operation of the actual remedial system. This upgradient propagation of the dissolved plume was also in contradiction with the simulated particles of groundwater started from the chlorobenzene source area, which were all captured downgradient of the source by CZ remedial wells and did not migrate upgradient into the area of the plume propagation. This further confirms that the simulated upgradient propagation of the plume in this area is an art-effect of numerical dispersion and should not be considered during the optimization runs.

• Plume volume reduction was evaluated separately for the MBFC and Gage aquifers after 10, 25, and 50 years of the implementation of remedial actions. The remediation target values used by PEST were set to match the ROD requirements listed above. The targets were set in such a manner that faster plume removal than specified in the ROD was permitted without penalty. Annual plume-reduction targets, which were not required by the ROD, were added by linearly interpolating between the 10-, 25-, and 50-year targets to facilitate the optimization process. The annual targets were weighted less than the 10-, 25-, and 50-year targets required by the ROD.

Plume reduction was considered successful if the 10-, 25-, and 50-year targets were achieved, or if more plume reduction than required by the ROD was achieved at those times. If the plume reduction targets were not achieved, it resulted in a larger (less-desirable) objective function. Consequently, the remedial wellfield was adjusted for the subsequent optimization simulations to improve the remedial performance with regard to the plume reduction targets.

Pore-Volume Flushing

As discussed in the ROD, flushing of the aquifer is the process by which contaminants are pushed from the ground during hydraulic extraction of groundwater. Greater pore-volume flushing should result in a more rapid exchange of groundwater through the contaminated area, producing faster cleanup. The ROD specifies that the remedial actions shall be designed in such a way that, when modeled by the EPA-approved RD model:

- At least one net pore volume of water per year be exchanged throughout the area of the above-ISGS concentrations of chlorobenzene outside the CZ in the MBFC and Lynwood aquifers.
- At least 0.5 net pore volume of water per year be exchanged throughout the area of above-ISGS concentrations of chlorobenzene outside the CZ in the Gage aquifer.

The pore-volume flushing rate target was estimated as follows:

- A computer program, similar to that used for the JGWFS analysis, was created to
 calculate pore-volume flushing rates within the chlorobenzene plume outside the CZ.
 Although this method of estimating pore-volume flushing rates is based on the
 volumetric flux and represents a significant simplification of the natural system, it was
 used for this analysis to be consistent with the estimates performed for the JGWFS,
 which served as a basis for the ROD requirements.
- The minimum, maximum, and mean pore-volume flushing rates were estimated for the MBFC and Gage aquifers.
- The remediation target values for pore-volume flushing rates used by PEST were set to match the performance criteria specified in the ROD and listed above. The targets were set such that higher pore-volume flushing rates than those specified in the ROD did not result in a penalty.

Pore-volume flushing was considered successful for each stress period if the rates required by the ROD were achieved and/or exceeded. Less pore-volume flushing than the target values resulted in a larger (less-desirable) objective function. This target had lower weighting, however, than the plume containment and plume reduction targets, to ensure

that achieving pore-volume flushing did not take pre-eminence over other performance criteria.

Limiting Adverse Migration Targets

As discussed in the ROD, the remedial action shall limit the adverse migration of NAPL and dissolved-phase contaminants. The ROD requires that the RD should be adjusted to prevent or reverse adverse migration, but limiting adverse migration shall not take preeminence over other remediation objectives specified in the ROD and discussed above. Consequently, the adverse migration should be limited without reducing the pumping rates of wells required to meet the other ROD objectives. This may include potentially adding containment wells in the impacted areas to offset adverse migration.

The remediation targets that were developed for limiting adverse migration include targets for NAPL and dissolved-phase contamination. Both of these targets are discussed below.

Limit Adverse Migration of NAPL

The ROD requires that the remediation actions limit downward migration of NAPL by limiting drawdown and changes in vertical gradients in the physical space where NAPL occurs. In order to steer the optimization process toward the remedial wellfield that is less likely to mobilize NAPL, a remediation target for minimum increase in vertical gradients within the CZ, where NAPL occurs, was incorporated into the optimization simulations. Incorporation of the remediation target for minimum increase in vertical gradients into the model was accomplished as follows:

- A computer program was developed that calculates the maximum vertical head difference between source areas defined in the CZ and an underlying aquifer including:
 - Between the UBF and the MBFC
 - Between the MBFB and the MBFC
 - Between the MBFC and Gage aquifers
- The remediation target values for the vertical gradients used by PEST were set to less than or equal to the values of ambient gradients simulated under nonpumping conditions.

Limiting adverse migration of NAPL was considered successful for each stress period if the downward gradients in NAPL areas were not increased. This target had lower weighting with regard to its contribution to the objective function than the plume containment and plume reduction targets, to ensure that limiting adverse migration did not take preeminence over other performance criteria.

Limit Adverse Migration of Dissolved Contamination

The ROD requires that the remedial action shall be designed to limit adverse migration of dissolved contaminants within the context of meeting all other provisions of the ROD. Adverse migration of dissolved contaminants is defined as movement of chlorobenzene, benzene, and TCE plumes to areas that are not presently affected by these plumes. To account for adverse migration, an additional remediation target referred to as "newly contaminated area" was incorporated into the model as follows:

- The newly contaminated area was calculated as the total area of model cells that exceed ISGS levels for the current year, but did not at the previous year. The newly contaminated area was calculated for each year, for each aquifer.
- The optimization target value used by PEST for the newly contaminated area was set to zero square feet (i.e., no increase in contaminated area).

As discussed above, this target also was used for assessing capture of the overall distribution for benzene. This target had lower weighting with regard to its contribution to the objective function than the chlorobenzene plume containment and reduction targets; this was intended to ensure that limiting adverse migration did not take pre-eminence over other performance criteria. Specifically, this lower weighting was performed in order to prevent the need for reducing the aggressiveness of the chlorobenzene remedy in order to minimize the adverse migration of other contaminants such as benzene and TCE. Instead, it was assumed that additional pumping and/or injection would be added to the remedial wellfield, if required, to capture the areas impacted by adverse migration of these contaminants and pull these contaminants back into the CZ.

Redistribution of Groundwater Extraction

As discussed in the ROD, the volume of groundwater that is contaminated above ISGS concentrations will shrink during chlorobenzene plume reduction, and the downgradient portion of the plume will be eliminated before the portion of the plume located more proximally to the NAPL sources. As the plume shrinks, the most downgradient hydraulic extraction wells will come to be located outside of the plume area. If the pumping outside the plume were to continue, these wells would counter further progress in shrinking the plume as they pull contaminants back into previously treated areas. To avoid this in practice (and correspondingly in the design of the modeling simulations), pumping from these wells is discontinued (turned off) at appropriate points in time as the plume shrinks and extraction wells come to lie outside the remaining plume area. The ROD requires that pumping from such deactivated wells be reallocated (if necessary) to extraction wells still being pumped inside the remaining plume area. Consequently, the reconfiguration of the initial wellfield with the subsequent redistribution of flow among the remaining wells needs to take place in the course of the remedial actions.

In general, the more pumping from the deactivated wells is redistributed among the remaining wells, the more rapid cleanup of the remainder of the plume would occur outside the CZ. However, the reallocation of too much pumping to wells located near the CZ could cause a breach of CZ containment, which is prohibited by the ROD. This breach of containment, in turn, would complicate and very likely impede the cleanup of the remainder of the plume outside the CZ. Attempting to counter such a breach by increasing extraction from the CZ wells to reestablish hydraulic control of the CZ is not practical, because groundwater extraction from these wells is limited by aquifer hydraulic properties. In addition, the increase in extraction from the CZ wells could potentially mobilize DNAPL. Therefore, the redistribution of pumping was simulated and optimized so as to achieve a balance between the ROD goals of (1) redistributing as much flow as possible from deactivated wells to minimize the cleanup time, and (2) maintaining hydraulic containment of the CZ.

To achieve this balance, the optimization process included the reduction of the total pumping rate of the remedial wellfield, if redistributed flow would cause the breach of CZ containment. As a result, the optimized total extraction rate of the remedial wellfield decreased as more wells became deactivated, while the flow rates of remaining individual wells increased (see Section 4.2, Table 4-3).

The optimization process was designed to account for the wellfield reconfiguration and redistribution of flow each time one or more wells achieved threshold (i.e., target shutdown) concentrations (see Section 4.2.1). The fraction of redistributed flow was optimized for each reconfigured wellfield to achieve the ROD objectives. As the simulated concentrations in extraction wells dropped below a threshold concentration, the wells were deactivated, and the remaining wells were optimized.

In order to implement an automatic optimization of the flow redistribution, a command (batch) file was developed and used for running multiple model runs using both MODFLOW and MT3DMS. The command file was written so that the model run was stopped each time the concentration in any of the extraction wells dropped below a threshold concentration. The threshold concentration was adjusted during PEST simulations to optimize achievement of the ROD requirements. For each subsequent model run, all wells in which concentrations dropped below the threshold concentration were shut down and pumping was redistributed among the remaining wells. The final concentrations from the previous run were used as initial concentrations for the subsequent run. These model runs were repeated until the plume reduction requirement in the ROD was met.

Some modifications to the MT3DMS code were made to minimize the amount of time required for the model flow redistribution runs. Ordinarily, MT3DMS halts a run after a specified duration of simulated time. In the case of flow-redistribution runs, it was impossible to determine in advance how long each run should continue before one or more wells reached threshold concentrations. This could result in extensive wasted computing time; for example, if a 30-year run time is specified and the concentrations in wells drop below the threshold after 10 years, computing time for the final 20 years would be wasted. The MT3DMS code was modified to allow automatic termination of the model run after one or more wells achieve the threshold concentrations. Modifications to the MT3DMS code are described in Appendix C.

The redistribution of flow between the wells was performed as follows:

- Constant pumping rates were assigned directly to the CZ containment extraction wells, and to the TCE containment wells.
- The CZ containment well pumping and TCE pumping was subtracted from the total optimized flow rate of the remedial wellfield, and the fractions of the remaining flow were redistributed among the wells outside the CZ to achieve the ROD requirements.
- The redistribution process was repeated each time when one or more wells were shutdown, and the additional flow from deactivated wells was redistributed among the remaining wells. As discussed in Section 4.1, the optimization process was focused on minimizing the objective function by identifying the pumping and injection rates in individual wells that were required to meet the ROD requirements. As a result, the

additional redistributed flow was reduced as necessary by the optimization process to prevent breach of the CZ containment.

- A similar fraction-assignment process was used to assign flow rates to injection wells.
- The optimized total flow for each wellfield configuration was calculated as the initial total flow, minus the flow from deactivated wells, plus the reallocated portion of flow from deactivated wells.

This flow redistribution process ensures that remedial extraction remains optimized as the size and the shape of the plume changes in the course of remedial actions.

4.1.2 Remedial Design Constraints

The RD must be constrained by realistic physical limitations, such as maximum capacities of extraction and injection wells, and realistic locations for pumping and injection wells, which consider access restrictions and other considerations. For the purposes of automatic optimization, these constraints had to be translated into numerical equivalents and incorporated into the model, so that unrealistic well locations and pumping/injection rates were eliminated from consideration. A brief description of the implementation of each RD constraint is provided below.

Locations of Extraction and Injection Wells

Because the remedial wellfield will be installed in a developed area, limited locations are available for extraction and injection wells. Initial wellfield configuration was developed in consultation with Shell and Montrose based on the October 2006 distribution of contaminant concentration data, and available data regarding the access restrictions.

The initial configuration of the remedial wellfield included a relatively small number of injection and extraction wells in order to reduce the number of stagnation zones within the plume. In general, any two extraction wells in the same aquifer will have a stagnation zone between them, which can slow the rate of plume reduction. Because of this, using only as many extraction wells as necessary to achieve the ROD requirements and maintaining the right balance between the factors listed above and the reliability of the remedial wellfield is preferred to operating more wells. In addition, this approach improves the implementability and cost-effectiveness of the remedy. In the process of optimization, the well locations were further adjusted, and several extraction and injection wells were added to the remedial wellfield in order to improve the wellfield performance with regard to meeting the remediation targets (see Section 4.2). Access restrictions and other factors were also considered for these additional wells.

Maximum Capacities of Wells

Maximum capacities of individual extraction and injection wells were estimated by H+A based on the results of pilot test data at installed wells, and from aquifer characteristics at proposed well locations. The flow rates of individual wells were limited in the optimization process by these maximum capacities. If the ROD requirements could not be achieved with all wells operating at or below their maximum capacities, additional well locations were added, and the system was optimized again.

4.1.3 Optimization Target

As discussed above, the ROD requires a minimum pumping rate of 700 gpm for the remedial wellfield. Consequently, the pumping rate optimization target was set up to 700 gpm, and the optimization process was used to identify the most efficient distribution of pumping that can achieve the ROD requirements at a flow rate that is as close as possible to, but not less than, 700 gpm.

The pumping rate optimization target for the remedial wellfield was incorporated into optimization simulations as a "soft" target, compared to the "hard" remediation targets such as plume volume reduction, plume containment, etc. This means that given similar performance in achieving remediation targets, the wellfield that meets the pumping rate optimization target would be selected.

4.2 Remedial Wellfield Optimization Results

This section discusses the results of the remedial wellfield optimization including (1) specifications for the optimized remedial wellfield, which were used to develop an OOD, and (2) comparison of the simulated wellfield performance to the remediation targets discussed in Section 4.1.1. The OOD is discussed in detail in the Overall Operational Design Report (CH2M HILL, 2008). Appendix A contains a DVD with an electronic copy of the complete set of optimized wellfield simulations using the calibrated RD model.

4.2.1 Specifications for the Optimized Remedial Wellfield

The specifications for the optimized remedial wellfield discussed below include the following:

- 1. Locations and rationale for the extraction and injection wells in the overall system (in both areal dimensions and depth/HSU dimensions), as well as the approximate number of extraction and injection wells based on the assumed or estimated well capacities;
- 2. Optimized flow rates of the remedial wellfield including the initial total pumping rate of the remedial wellfield, initial rates of extraction and injection wells, and maximum flow rates of individual wells;
- 3. Operational considerations for the remedial wellfield including concentration target shutdown levels for shutting down extraction wells, general guidance for redistributing flow between the wells, and considerations pertaining to operation of the wells involved in maintaining containment of the CZ as specified in the ROD; and
- 4. Estimated (modeled) influent concentrations of chlorobenzene, benzene, and p-CBSA, including flow-weighted average concentrations and well-specific concentrations.

Please note that engineering specifications for wells, conveyances, or treatment systems, including materials, conveyance alignments, injection controls, equipment, systems design, or any other such engineered characteristics were not included in the scope of these modeling activities. The specifications for the optimized remedial wellfield discussed in this section also do not include contingencies that should be incorporated in the formal design due to uncertainty in future operational needs and conditions. It also should be recognized that

these specifications were developed based on the currently available information, and as new information is obtained—especially field operational data during remedy implementation—the wellfield may need to be reoptimized and adjusted to ensure compliance with ROD requirements (for instance, modifying pumping rates and/or adding wells).

Locations and Approximate Number of Extraction and Injection Wells

This section presents the optimized locations for the remedial wells, including both extraction and injection wells. One well per location was assumed for the purposes of this optimization effort. This assumption was made based on the available data regarding the hydrogeologic properties of the formation and the estimated capacities of the existing wells (i.e., based on the design constraints). However, if it is determined during the design or remedy implementation that the required flow rate cannot be achieved at certain locations with just one well, additional wells will need to be installed at these locations to meet the requirements of the ROD. These additional wells should be installed in the general vicinity of the proposed locations, but at a sufficient distance from existing extraction and/or injection wells to avoid interference between the wells (i.e., significant impact on drawdown or buildup in the adjacent wells).

Figures 4-1A through 4-1C show the locations of the remedial wells, including injection and extraction wells in the water table, MBFC, and Gage aquifers. The coordinates of these wells are presented in Table 4-1. The overall optimized remedial wellfield includes a total of 17 extraction wells (3 wells in the water table aquifer, 7 wells in the MBFC, and 7 wells in the Gage aquifer), and 6 injection wells (3 wells in the MBFC and 3 wells in the Gage aquifer). Of these wells, 6 extraction wells and 4 injection wells have already been installed as part of the pilot testing program (Figures 4-1A through 4-1C).

TABLE 4-1
Coordinates of Proposed Locations for Extraction and Injection Wells

Well-ID	Easting (feet)	Northing (feet)
UBA-EW-A	4196962	4056685
UBA-EW-B	4197737	4056797
MBFB-EW-1	4197447	4056528
BF-EW-1	4197422	4056537
BF-EW-2	4198681	4054093
BF-EW-B	4197901	4055049
BF-EW-D	4199017	4053193
BF-EW-M	4196962	4056685
BF-EW-N	4197737	4056797
BF-EW-TCE	4197700	4058500
G-EW-1	4197413	4056557
G-EW-2	4199810	4053771
G-EW-3	4197124	4054177

TABLE 4-1
Coordinates of Proposed Locations for Extraction and Injection Wells

Well-ID	Easting (feet)	Northing (feet)
G-EW-B	4198806	4055526
G-EW-E	4200180	4053281
G-EW-O	4198712	4054397
G-EW-TCE	4197700	4058500
BF-IW-1	4194654	4057024
BF-IW-2	4200276	4054984
BF-IW-E	4194114	4057626
G-IW-1	4194654	4057065
G-IW-2	4199886	4056660
G-IW-D	4199664	4057762

Note:

Datum used for well coordinates is MNAD27 (Modified State Plane Zone VII NAD 27 feet).

As discussed above, the initial locations for the remedial wells were selected based on the configuration of the contaminant plumes and site access considerations. The CZ extraction wells are located in each impacted aquifer (i.e., water table aquifer, MBFC, and Gage aquifer) within the CZ, downgradient of the source area. The plume-reduction wells, in general, are located along the central axis of the contaminant plumes. The well locations were refined based on the optimization process in order to achieve the requirements and standards of the ROD. For example, the locations of the plume-reduction wells were adjusted and moved further downgradient from the CZ so that these wells would not interfere with the CZ containment wells (i.e., would not pull contaminated groundwater out of the CZ).

The optimization process resulted in adding several extraction and injection wells to the remedial wellfield. Wells BF-EW-M and BW-EW-N were added to improve the CZ containment in the MBFB aquifer (Figure 4-1A). Additional extraction well G-EW-E was added at the toe of the chlorobenzene plume in the Gage aquifer in order to meet the ROD requirement for the overall chlorobenzene plume containment and volume reduction (Figure 4-1C). A failure of plume containment in this area would pose a significant risk to downgradient receptors and may cause rapid migration of contaminants both laterally and vertically. The Gage aquifer is a drinking water aquifer and several municipal wells are located in relatively close proximity to the toe of the chlorobenzene plume. The hydraulic gradient is significantly steeper at the downgradient edge of the chlorobenzene plume in the Gage aquifer, possibly due to the impact of the downgradient municipal extraction. This makes hydraulic containment more difficult. Any potential increase in downgradient extraction from the municipal wells could result in further increase of the hydraulic gradient and greater loss of plume containment. Because the existing downgradient well, G-EW-2,

has a limited specific capacity (see Section 4.2.1.2), an additional extraction well in this area is critical for the reliable containment and subsequent success of the remedy.

Also as a result of the optimization process, the locations and flow rates of injection wells were adjusted and one well was added to the remedial wellfield in order to reduce the adverse impact of remedial pumping on other contaminant plumes such as the TCE and benzene plumes. As a result, injection at the Del Amo site will be performed in two Gage injection wells (existing well G-IW-2 and new well, G-IW-D, which was added during optimization) in order to reverse the downward gradient between the MBFC and Gage aquifers in the area where elevated concentrations of benzene and TCE are present in the MBFC (Figure 4-1C). Reversing the downward hydraulic gradient in this area will prevent the vertical migration of TCE and benzene into the Gage aquifer and will ensure containment of these contaminants within the CZ in the MBFC.

The primary rationale for the locations of each extraction and injection well is presented in Table 4-2.

TABLE 4-2
Rationale for Locations of Remedial Wells

Location	Rationale
MBFB-EW-1	Containment of the chlorobenzene plume within the CZ in the water table aquifer
UBA-EW-A	Containment of the chlorobenzene plume within the CZ in the water table aquifer
UBA-EW-B	Containment of the chlorobenzene plume within the CZ in the water table aquifer
BF-EW-1	Containment of the chlorobenzene plume within the CZ in the MBFC
BF-EW-M	Containment of the chlorobenzene plume within the CZ in the MBFC
BF-EW-N	Containment of the chlorobenzene plume within the CZ in the MBFC
BF-EW-B	Reduction of the chlorobenzene plume outside the CZ in the MBFC
BF-EW-2	Reduction and containment of the chlorobenzene plume outside the CZ in the MBFC
BF-EW-D	Reduction and containment of the chlorobenzene plume outside the CZ in the MBFC
BF-EW-TCE	Containment of the TCE plume migration from upgradient sources in the MBFC
G-EW-1	Containment of the chlorobenzene plume within the CZ in the Gage aquifer
G-EW-B	Reduction and containment of the chlorobenzene plume outside the CZ in the Gage aquifer
G-EW-3	Reduction and containment of the chlorobenzene plume outside the CZ in the Gage aquifer
G-EW-O	Reduction and containment of the chlorobenzene plume outside the CZ in the Gage aquifer
G-EW-2	Reduction and containment of the chlorobenzene plume outside the CZ in the Gage aquifer
G-EW-E	Reduction and containment of the chlorobenzene plume outside the CZ in the Gage aquifer
G-EW-TCE	Containment of the TCE plume migration from upgradient sources in the Gage aquifer
BF-IW-1	Disposal of treated groundwater and mitigation of adverse TCE migration from upgradient sources in the MBFC
BF-IW-E	Disposal of treated groundwater and mitigation of adverse TCE migration from upgradient sources in the MBFC
BF-IW-2	Disposal of treated groundwater and flushing the plume toward extraction wells in the MBFC
G-IW-1	Disposal of treated groundwater and mitigation of adverse TCE migration from upgradient sources in the Gage aquifer
G-IW-2	Disposal of treated groundwater and maintaining upward gradient between the Gage aquifer and MBFC to prevent vertical migration of benzene into the Gage aquifer (i.e., contain benzene within the CZ)
G-IW-D	Disposal of treated groundwater and maintaining upward gradient between the Gage aquifer and MBFC to prevent vertical migration of benzene into the Gage aquifer (i.e., contain benzene within the CZ)

Optimized Flow Rates of the Remedial Wellfield

This section discusses the optimized flow rates for the remedial wells, including the total pumping rate of the initial remedial wellfield, the initial rates of individual extraction and injection wells, and the maximum flow rates of individual wells.

Total Flow Rate of Initial Remedial Wellfield(s)

Based on the optimization modeling, a total extraction rate of 729 gpm is required to achieve the ROD standards (Table 4-3). This includes extraction of 700 gpm to address the ROD standards for the chlorobenzene and benzene plumes, and extraction of 29 gpm to address the ROD standards for the TCE plume.

Initial Flow Rates of Individual Wells

The optimized flow rates for extraction and injection are included in Table 4-3. These include the initial flow rates and subsequent redistribution of pumping and injection after the concentrations in some wells decrease below threshold shutdown levels and those wells are shut down. The initial flow rates of wells are also shown in Figures 4-1A through 4-1C for the water table, MBFC, and Gage aquifers.

Maximum Flow Rates of Individual Wells

The maximum rates for individual wells are provided in Table 4-3. For some extraction wells, the maximum rates are higher than the initial rates, because additional pumping may need to be added to those wells as part of pumping redistribution to meet ROD standards after shutting down the wells that have achieved threshold concentration levels. Consequently, the RD should ensure that the wells have sufficient capacity to achieve these rates, if required. For injection wells, the maximum flow rates shown are the same as the initial rates.

Based on pilot testing data presently available, existing wells appear to have sufficient capacity to achieve maximum flow rates, if required (Table 4-3). However, actual field conditions may differ from previously estimated values. Consequently, additional contingency should be considered for the design of remedial wells. Further, the maximum flow rates discussed in this report should not define the capacity of the treatment system and conveyances. As discussed above, treatment system capacity should be designed with a sufficient margin of contingency due to uncertainty in future operational needs and conditions.

Operational Considerations for the Remedial Wellfield

The ROD requires reduction in the volume of the chlorobenzene plume outside the CZ to zero over time. The optimization process accounted for this by simulating shutdown of remedial extraction wells at the simulated time when the contaminant concentrations in these wells decreased below a certain threshold level, as explained below. This threshold level is referred to as the "target shutdown level" in the following discussion.

TABLE 4-3 Optimized Flow Rates for Remedial Wells

Optimized !	low Rates for Reme	uidi IVollo	Time Peri	iod/Duration	(years)			
		Initial Flow	Redistribu	tion of Pump Start Shutt	Maximum Flow			
Aquifer	Well Identification	Rates (0 to 15)	15 – 18/ 3	18 – 26/ 8	26 – 30/ 4	30 – 32/ 2	Rate (gpm)	Estimated Capacity
			Extraction	Well Rates (gpm)			
	UBA-EW-A	6.0	6.0	6.0	6.0	6.0	6.0	12
Water Table	UBA-EW-B	12.0	12.0	12.0	12.0	12.0	12.0	24
	MBFB-EW-1*	4.0	4.0	4.0	4.0	4.0	4.0	4
	BF-EW-1*	35.0	35.0	35.0	35.0	35.0	35.0	35
	BF-EW-2*	67.6	68.5	75.1	77.0	79.9	79.9	90
	BF-EW-B	63.9	64.8	71.0	72.9	75.6	75.6	80
MBFC	BF-EW-D	132.4	134.2	Well shut down	Well shut down	Well shut down	134.2	140
	BF-EW-M	35.0	35.0	35.0	35.0	35.0	35.0	NA
	BF-EW-N	35.0	35.0	35.0	35.0	35.0	35.0	NA
	BF-EW-TCE	12.0	12.0	12.0	12.0	12.0	12.0	NA
	G-EW-1*	120.0	120.0	120.0	120.0	120.0	120.0	250
	G-EW-2*	29.5	29.9	32.7	33.6	Well shut down	33.6	70
	G-EW-3*	24.9	25.3	27.7	Well shut down	Well shut down	27.7	30
Gage	G-EW-B	57.1	57.9	63.5	65.1	67.6	67.6	80
	G-EW-E	29.5	Well shut down	Well shut down	Well shut down	Well shut down	29.5	50
	G-EW-O	48.1	48.7	53.4	54.8	56.8	56.8	60
	G-EW-TCE	17.0	17.0	17.0	17.0	17.0	17.0	NA
	action Rate of lial Wellfield	729.0	705.4	599.4	579.5	555.9		
			Injection \	Nell Rates (g	gpm)			
	BF-IW-1*	39.9	38.6	32.6	31.4	30.1	39.9	130
MBFC	BF-IW-2*	39.9	38.6	32.6	31.4	30.1	39.9	150
	BF-IW-E	56.8	54.8	46.3	44.7	42.7	56.8	70
	G-IW-1*	312.5	302.0	254.8	245.9	235.3	312.5	610
Gage	G-IW-2*	125.4	121.2	102.2	98.7	94.5	125.4	350
	G-IW-D	125.4	121.2	102.2	98.7	94.5	125.4	260

Note:
* Wells installed for pilot testing

As the simulation proceeded after the shutdown, the flow was then redistributed among the remaining extraction wells. Considering the redistribution of flow (pumping) in the optimization process allowed for the more effective use of extraction wells and resulted in a lower optimized total flow rate for the remedial wellfield than that estimated without considering flow redistribution. Further evaluation of the optimized flow redistribution in modeling runs indicated that the following aspects pertaining to the operation of the remedial wellfield should be considered and accounted for during the RD and remedy implementation:

- Target shutdown levels for extraction wells
- General guidance for redistributing flow between the wells
- Operation of CZ containment wells

Target Shutdown Levels for Extraction Wells

The optimization simulations of the remedial wellfield indicated that the target shutdown level for contaminant concentrations, at which extraction wells can be turned off, is an important parameter that should be considered for the development of the performance monitoring program and during remedy implementation. Specifically, the modeling results indicated that shutting off extraction wells at concentrations equal to the ISGS level for chlorobenzene (70 µg/L) would result in a loss of hydraulic containment for part of the chlorobenzene plume. As this uncaptured portion of the plume migrates downgradient, previously cleaned areas of the aquifer would become recontaminated. This is because the need for downgradient containment is not eliminated when the contaminant concentration in a plume-reduction well reaches the ISGS level. For example, an extraction well located at the toe of the chlorobenzene plume could extract groundwater from both upgradient locations with contaminant concentrations above the ISGS and from downgradient locations where groundwater is already below ISGS levels. In this example, the resulting diluted contaminant concentrations in the well could be below the ISGS levels; however, if this well is shut off, the above-ISGS concentrations from the upgradient areas can escape the extraction system.

Based on the modeling optimization runs, using a target shutdown level of 10 to 15 μ g/L of chlorobenzene is more appropriate than the ISGS level, because it does not result in the contaminant plume escaping downgradient containment. A detailed discussion pertaining to the monitoring and sampling procedures required for shutting down remedial wells, and the rationale for the concentration target shutdown levels will be included in the Monitoring and Compliance Plan (MACP), which will be prepared in 2008.

Redistributing Flow

The modeled distribution of flow between the extraction and injection wells for five consecutive simulated time periods is presented in Table 4-3. The initial time period terminates after 15 years, when the concentration in well G-EW-E decreases below the target shutdown level of 10 μ g/L. The second time period starts with well G-EW-E being shut down and the flow from this well being redistributed between the remaining wells. The second time period and each subsequent time period also terminate when the concentrations in at least one extraction well drop below the target shutdown level. Each time, the flow is redistributed between the remaining wells in a manner that allows the most cost-effective achievement of ROD standards.

A number of operational issues have been identified by modeling in the process of the remedial wellfield optimization simulations; these issues should be considered during the design and operation of the remedial wellfield, and include the following:

- Additional pumping should not be redistributed to the CZ containment wells (unless
 monitoring during remedy implementation demonstrates the lack of capture) as it may
 induce horizontal and/or vertical gradients in the DNAPL source area.
- Flow redistribution should be performed in a manner that does not result in creating interference (i.e., competition for capture) between the CZ containment wells and the wells located downgradient of the CZ. The significant increase in flow rates in wells located downgradient of the CZ containment wells may cause a loss of capture in the CZ and result in contaminated groundwater bypassing CZ containment wells and migrating toward the wells with increased extraction. Consequently, only a portion of the flow from the cleaned up wells may need to be redistributed between the remaining wells. Additional modeling runs using the revised numerical model of the Dual Site should be performed each time the flow from clean wells needs to be redistributed between the remaining wells to optimize the performance of the remedial wellfield.
- The optimized amount of injection into the Gage aquifer significantly exceeds injection into the MBFC. This distribution of injection helps to mitigate the adverse vertical migration of DNAPL and dissolved contaminants into the Gage aquifer. When the amount of water available for injection decreases because of reduced extraction, injection in the MBFC wells should be stopped or reduced first. Injection in the Gage well located west of the Montrose site (well G-IW-1) can be reduced with further reduction of pumping. However, injection rates should be maintained at Gage injection wells (G-IW-2 and G-IW-D) located at the Del Amo site to prevent vertical migration of TCE and benzene from the CZ in the MBFC into the Gage aquifer.

Operation of CZ Containment Extraction and Injection Wells

Most plume-reduction wells will be shut down after meeting the ROD requirements. However, as required by the ROD, the CZ containment wells will operate indefinitely or until the sources of contamination are removed and the groundwater within the CZ is remediated. This includes the CZ containment extraction wells UBA-EW-A, MBFB-EW-1, and UBA-EW-B in the water table aquifer; BF-EW-1, BF-EW-M, and BF-EW-N in the MBFC; and G-EW-1 in the Gage aquifer. In addition, Gage injection wells G-IW-2 and G-IW-D are also considered to be CZ containment wells because these wells prevent vertical migration of TCE and benzene from the CZ in the MBFC into the Gage aquifer (Table 4-2). Extraction and injection rates of the CZ containment wells can be adjusted upon shutting down other remedial extraction wells. It is expected that the amount of extraction from the CZ containment wells will be sufficient to maintain adequate injection into the CZ injection wells at the Del Amo site.

It is assumed for the purposes of this RD, that the TCE containment wells BF-EW-TCE and G-EW-TCE also will operate indefinitely or until the upgradient sources of contamination are removed and the groundwater at the upgradient locations is remediated. Additional modeling runs using the revised numerical model of the Dual Site can be performed to determine the flow rates of the CZ containment wells and TCE containment wells when the

chlorobenzene plume-reduction wells achieve cleanup standards and are no longer in operation.

Simulated Treatment System Influent Concentrations

Simulated influent concentrations of chlorobenzene, benzene, and p-CBSA for each well are presented in Tables 4-4 through 4-6. These tables also present the flow-weighted average concentration for each of these constituents. The estimates of contaminant concentrations are presented for a simulated duration of remedial action of 32 years. Modeling results indicate that the ROD requirements pertaining to the reduction of the chlorobenzene plume will be met after 32 years and most remedial wells will be shut down at that time. The CZ containment wells will be in operation indefinitely, and it can be assumed for the purposes of the design that the concentrations in these wells will stay constant.

While the estimates of contaminant concentrations presented in Tables 4-4 through 4-6 should be used for the design of the treatment facility, these estimates do not include the contingency that should be incorporated in the formal design due to uncertainty associated with modeling estimates of contaminant concentrations and future operational needs and conditions. In general, the early-time estimates of influent concentrations are expected to be more accurate than the late-time concentrations, because they are less impacted by the modeling uncertainties and uncertainties associated with future conditions.

The influent concentrations of TCE are not presented in this report, because modeling of the solute transport of TCE was not included in the scope of optimization modeling (see Sections 2 and 3).

4.2.2 Comparison of Simulated Wellfield Performance to Remediation Targets

This section presents a comparison of the performance of the optimized remedial wellfield to the remediation targets (i.e., the ROD requirements). As discussed in Section 4.1, these requirements include:

- Minimum total pumping rate of the remedial wellfield
- Indefinite containment within the CZ
- Containment of the overall contaminant distribution
- Reduction of the volume of water with concentrations of contaminants above drinking water standards to zero within certain timeframes
- Certain pore-volume flushing rates within the contaminant distribution
- Limiting adverse migration of contaminants
- Redistribution of groundwater extraction as the contaminant plume shrinks

TABLE 4-4
Simulated Chlorobenzene Influent Concentrations

	Simulated Chlorobenzene Influent Concentrations (µg/L)															
Elapsed Time (years)	Flow-Weighted Average Concentration (µg/L)	UBA-EW-A	UBA-EW-B	MBFB-EW-1	BF-EW-1	BF-EW-2	BF-EW-B	BF-EW-D	BF-EW-M	BF-EW-N	G-EW-1	G-EW-2	G-EW-3	G-EW-B	G-EW-E	G-EW-O
0	7,711	1,746	4,449	2,010	22,974	17,361	11,677	1,838	28,912	19,003	4,581	294	660	1,595	236	179
1	4,490	13,172	3,565	7,275	17,199	8,882	6,250	1,405	12,556	7,044	3,094	157	910	1,915	167	114
2	3,242	21,038	3,050	12,017	12,522	4,938	4,287	880	7,625	5,775	2,470	118	927	1,674	126	105
3	2,648	25,533	2,593	16,388	9,731	2,865	3,076	543	6,265	5,147	2,416	94	896	1,371	96	114
4	2,306	27,723	2,246	20,196	8,079	1,744	2,238	339	5,825	4,726	2,398	76	842	1,095	75	132
5	2,091	28,615	2,029	23,491	7,071	1,120	1,630	217	5,658	4,426	2,370	64	775	873	59	157
6	1,953	28,892	1,942	26,399	6,443	759	1,181	144	5,584	4,213	2,341	54	700	701	47	184
7	1,863	28,937	1,970	29,019	6,044	538	850	99	5,548	4,062	2,318	46	621	570	38	212
8	1,805	28,929	2,083	31,401	5,790	395	610	70	5,527	3,958	2,300	40	540	466	31	239
9	1,769	28,926	2,252	33,547	5,627	297	437	52	5,514	3,886	2,286	35	460	385	25	264
10	1,746	28,937	2,450	35,443	5,521	228	315	40	5,504	3,835	2,276	31	386	320	21	286
11	1,732	28,949	2,651	37,074	5,452	177	229	31	5,497	3,800	2,269	28	318	267	17	304
12	1,723	28,950	2,840	38,435	5,405	139	170	25	5,490	3,775	2,263	25	258	223	15	318
13	1,717	28,930	3,008	39,537	5,374	111	129	21	5,485	3,758	2,259	23	207	186	12	326
14	1,712	28,888	3,151	40,401	5,351	91	100	17	5,479	3,745	2,256	21	164	156	11	329
15	1,708	28,823	3,268	41,058	5,335	75	80	15	5,475	3,736	2,254	19	129	131	9	327
16	1,759	28,815	3,346	41,345	5,295	62	66	13	5,480	3,696	2,247	16	100	110	9	315
17	1,753	28,744	3,408	41,592	5,283	53	56	11	5,480	3,684	2,246	14	78	92	9	301
18	1,748	28,650	3,458	41,748	5,274	46	49	10	5,477	3,677	2,245	13	60	77	9	283
19	2,021	28,839	3,376	39,847	5,010	35	40	7	5,445	3,464	2,227	14	45	71	9	256
20	2,005	28,831	3,340	39,179	4,975	31	34	5	5,442	3,426	2,229	14	34	60	9	229
21	1,994	28,755	3,329	38,668	4,960	27	30	4	5,440	3,409	2,231	14	26	51	9	203
22	1,985	28,652	3,327	38,241	4,951	25	27	3	5,437	3,402	2,232	14	20	43	9	178
23	1,977	28,539	3,327	37,880	4,945	23	24	2	5,435	3,397	2,232	14	16	37	8	154
24	1,970	28,425	3,327	37,576	4,940	21	22	2	5,433	3,395	2,232	13	13	32	8	133
25	1,963	28,315	3,327	37,324	4,935	20	21	2	5,431	3,393	2,231	12	10	28	8	114
26	1,958	28,210	3,327	37,115	4,932	18	19	1	5,428	3,392	2,231	12	8	24	8	97
27	2,009	27,827	3,357	36,766	4,893	17	18	1	5,326	3,418	2,212	11	7	22	7	83
28	2,003	27,641	3,375	36,594	4,883	17	18	1	5,307	3,428	2,211	11	6	20	7	71
29	1,999	27,499	3,391	36,477	4,878	16	17	1	5,301	3,432	2,213	10	5	17	7	60
30	1,996	27,381	3,407	36,397	4,874	15	16	1	5,298	3,435	2,213	9	4	15	6	51
31	2,078	27,343	3,402	36,223	4,854	14	15	1	5,305	3,409	2,207	8	4	13	6	41
32	2,075	27,271	3,404	36,135	4,849	14	15	1	5,306	3,403	2,208	7	4	12	6	35

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TABLE 4-5 Simulated Benzene Influent Concentrations

Simulated D	Benzene Influent Concentrations Benzene Concentrations (µg/L)															
Elapsed Time (years)	Flow-Weighted Average Concentration (µg/L)	UBA-EW-A	UBA-EW-B	MBFB-EW-1	BF-EW-1	BF-EW-2	BF-EW-B	BF-EW-D	BF-EW-M	BF-EW-N	G-EW-1	G-EW-2	G-EW-3	G-EW-B	G-EW-E	G-EW-O
0	48	1,210	0	4,872	74	19	22	0	34	17	0	0	0	0	0	0
1	7.2	216	0	791	10	3	3	0	6	-15	0	0	0	2	0	0
2	3.1	139	0	257	5	1	1	0	4	-7	0	0	0	3	0	0
3	2.5	127	0	141	4	0	0	0	4	1	0	0	0	2	0	0
4	2.4	125	0	117	4	0	0	0	4	3	0	0	0	2	0	0
5	2.4	125	0	111	4	0	0	0	4	4	0	0	0	1	0	0
6	2.4	125	0	110	4	0	0	0	4	4	0	0	0	1	0	0
7	2.4	125	0	110	4	0	0	0	4	4	0	0	0	1	0	0
8	2.4	125	0	110	4	0	0	0	4	4	0	0	0	0	0	0
9	2.4	125	0	110	4	0	0	0	4	4	0	0	0	0	0	0
10	2.4	125	0	110	4	0	0	0	4	4	0	0	0	0	0	0
11	2.4	125	0	110	4	0	0	0	4	4	0	0	0	0	0	0
12	2.4	125	0	110	4	0	0	0	4	4	0	0	0	0	0	0
13	2.3	125	0	110	4	0	0	0	4	4	0	0	0	0	0	0
14	2.3	125	0	110	4	0	0	0	4	4	0	0	0	0	0	0
15	2.3	125	0	110	4	0	0	0	4	4	0	0	0	0	0	0
16	2.4	126	0	108	4	0	0	0	4	4	0	0	0	0	0	0
17	2.4	126	0	108	4	0	0	0	4	4	0	0	0	0	0	0
18	2.4	126	0	108	4	0	0	0	4	4	0	0	0	0	0	0
19	2.7	126	0	97	4	0	0	0	4	4	0	0	0	0	0	0
20	2.7	126	0	95	4	0	0	0	4	4	0	0	0	0	0	0
21	2.7	126	0	95	4	0	0	0	4	4	0	0	0	0	0	0
22	2.7	125	0	94	4	0	0	0	4	3	0	0	0	0	0	0
23	2.6	125	0	94	4	0	0	0	4	3	0	0	0	0	0	0
24	2.6	125	0	94	4	0	0	0	4	3	0	0	0	0	0	0
25	2.6	125	0	94	4	0	0	0	4	3	0	0	0	0	0	0
26	2.6	125	0	94	4	0	0	0	4	3	0	0	0	0	0	0
27	2.7	124	0	94	4	0	0	0	4	3	0	0	0	0	0	0
28	2.7	124	0	94	4	0	0	0	4	3	0	0	0	0	0	0
29	2.7	124	0	94	4	0	0	0	4	3	0	0	0	0	0	0
30	2.7	124	0	94	4	0	0	0	4	3	0	0	0	0	0	0
31	2.8	124	0	93	4	0	0	0	4	3	0	0	0	0	0	0
32	2.8	124	0	93	4	0	0	0	4	3	0	0	0	0	0	0

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TABLE 4-6 Simulated p-CBSA Influent Concentrations

Simulated p	p-CBSA Influent Concentrations p-CBSA Concentrations (μg/L)															
Elapsed Time (years)	Flow-Weighted Average Concentration (µg/L)	UBA-EW-A	UBA-EW-B	MBFB-EW-1	BF-EW-1	BF-EW-2	BF-EW-B	BF-EW-D	BF-EW-M	BF-EW-N	G-EW-1	G-EW-2	G-EW-3	G-EW-B	G-EW-E	G-EW-O
0	39,989	68,022	28,607	12,086	86,737	98,080	113,356	12,013	99,514	38,787	17,264	7,300	5,687	22,155	4,824	297
1	23,821	73,417	15,494	71,516	75,177	48,303	46,404	10,355	62,022	21,919	10,206	3,581	6,785	16,269	4,295	755
2	17,622	64,895	11,512	87,800	63,133	26,706	27,326	6,921	46,371	24,554	10,625	2,749	5,861	11,164	3,551	1,082
3	13,951	58,248	8,978	87,227	53,334	14,914	17,254	4,354	41,350	25,933	10,656	2,071	4,938	7,402	2,857	1,673
4	11,738	54,448	7,466	82,275	46,733	8,639	11,159	2,693	39,751	26,322	10,501	1,538	4,069	4,951	2,287	2,329
5	10,412	52,703	6,790	78,210	42,701	5,260	7,255	1,672	39,204	26,368	10,358	1,141	3,268	3,413	1,843	2,914
6	9,613	52,103	6,692	76,174	40,339	3,362	4,718	1,057	39,000	26,333	10,259	854	2,552	2,429	1,504	3,351
7	9,123	52,021	6,909	75,726	38,979	2,236	3,078	686	38,916	26,293	10,195	650	1,935	1,775	1,245	3,614
8	8,812	52,109	7,243	76,138	38,200	1,533	2,029	458	38,876	26,266	10,154	505	1,427	1,321	1,047	3,710
9	8,608	52,206	7,579	76,860	37,752	1,078	1,365	316	38,854	26,252	10,127	400	1,025	997	892	3,661
10	8,466	52,257	7,865	77,582	37,492	777	947	224	38,839	26,246	10,110	323	720	761	771	3,492
11	8,361	52,257	8,090	78,177	37,339	575	683	164	38,828	26,246	10,099	264	497	588	673	3,230
12	8,280	52,216	8,261	78,622	37,246	438	515	123	38,819	26,250	10,091	219	338	460	594	2,902
13	8,214	52,149	8,392	78,936	37,188	344	406	94	38,810	26,255	10,087	184	228	364	528	2,535
14	8,159	52,070	8,495	79,153	37,150	279	333	74	38,803	26,262	10,083	157	153	291	473	2,155
15	8,112	51,987	8,582	79,304	37,124	234	284	59	38,795	26,268	10,081	135	103	235	426	1,786
16	8,311	52,049	8,600	78,930	36,901	197	246	49	38,869	26,020	10,057	111	69	195	519	1,411
17	8,275	52,001	8,639	78,805	36,870	172	219	41	38,881	25,981	10,056	103	47	161	555	1,111
18	8,247	51,933	8,684	78,716	36,853	153	198	35	38,879	25,969	10,055	99	33	133	567	861
19	9,474	52,392	8,365	74,251	34,919	117	167	22	38,662	24,373	9,984	106	23	135	575	619
20	9,418	52,377	8,257	72,674	34,738	102	145	15	38,662	24,158	10,000	106	16	119	565	457
21	9,385	52,272	8,215	71,569	34,678	91	128	10	38,662	24,089	10,005	103	12	102	548	341
22	9,362	52,147	8,196	70,782	34,653	83	116	8	38,660	24,066	10,006	98	9	87	526	258
23	9,346	52,024	8,190	70,235	34,638	76	105	6	38,657	24,059	10,006	91	8	75	502	200
24	9,334	51,908	8,191	69,862	34,627	69	97	5	38,654	24,057	10,006	84	6	64	478	158
25	9,324	51,799	8,199	69,613	34,619	64	90	4	38,650	24,058	10,006	77	5	56	453	128
26	9,317	51,698	8,211	69,448	34,612	59	84	3	38,647	24,059	10,006	70	4	50	429	106
27	9,571	51,010	8,308	68,922	34,337	55	79	2	37,870	24,281	9,917	65	5	46	406	87
28	9,563	50,756	8,373	68,816	34,289	51	74	2	37,778	24,357	9,924	59	5	42	384	73
29	9,560	50,578	8,431	68,803	34,272	47	70	2	37,757	24,391	9,929	53	5	39	362	63
30	9,558	50,439	8,481	68,828	34,263	44	66	1	37,750	24,408	9,932	48	5	37	342	55
31	9,956	50,446	8,468	68,609	34,130	41	63	1	37,821	24,207	9,903	47	5	35	319	49
32	9,950	50,364	8,478	68,526	34,111	38	59	1	37,837	24,168	9,903	45	5	34	299	44

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The compliance of the optimized remedial wellfield with these targets is discussed below.

Containment of CZ and Overall Contaminant Distribution

Chlorobenzene

The optimized wellfield captures 100 percent of the chlorobenzene CZ, the overall chlorobenzene plume, and the area of TCE beneath the high-concentration sources at the PACCAR and APC properties. Figure 4-2A shows particle-tracking results illustrating hydraulic capture of these areas using the initial optimized wellfield. Figures 4-2B through 4-2E indicate that successful capture of the CZ and the overall distribution is maintained as the plume reduction progresses and wells that achieve target shutdown levels are deactivated.

Benzene

As discussed above, the benzene containment was evaluated using solute transport simulations because the transport of benzene is significantly impacted by the process of natural biodegradation. The results of the benzene solute transport simulations are discussed in Section 4.2.2.4. A three-dimensional animation of benzene plume behavior is presented in Appendix E.

Plume Reduction

The optimized wellfield achieves chlorobenzene plume-reduction targets at 10, 25, and 50 years in both the MBFC and Gage aquifers (Figures 4-3, and 4-4A through 4-4C). The optimized wellfield reduces the chlorobenzene plume in both aquifers faster than required by the minimum plume reduction standard, which is 50 years. As shown in these figures, the target of 99 percent plume reduction is achieved after 32 years versus 50 years. A three-dimensional animation of chlorobenzene plume reduction is presented in Appendix E.

Pore-Volume Flushing

The optimized wellfield achieves the pore-volume flushing ROD requirement throughout most of the MBFC and Gage plumes (Figures 4-5A and 4-5B). The exception to this is several very small areas (few model cells) with a lower flushing rate (i.e., stagnation areas), which occur between extraction wells. As shown in Figures 4-5A and 4-5B, only two model cells in the MBFC, and six model cells in the Gage aquifer did not meet the pore-volume flushing rate remediation targets. These areas of lower flushing rates comprise less than one-half of 1 percent of the total plume area.

Adverse Migration

NAPL

As discussed in Section 4.1, the remediation target for minimum increase in vertical gradients beneath NAPL areas was included in the optimization process to limit the adverse migration of NAPL in response to pumping. However, some increase in vertical gradients in NAPL areas could not be avoided in order to meet the remediation targets of plume reduction and containment. In the DNAPL source area, downward head differences increased by about 0.1 foot (from 0.2 to 0.3 foot) compared to the ambient (before remedial pumping) head difference between the water table and the MBFC aquifers. This increase is relatively small, but may still have some limited impact on the vertical migration of

DNAPL. In the LNAPL source area, downward head differences increased by about 0.3 foot (from 1.8 to 2.1 feet) from the ambient head difference between the water table and the MBFC aquifers (see Figure 4-6). This small change in vertical head differences is not expected to have a significant impact on LNAPL trapped below the water table.

The ambient downward head differences between the MBFC and Gage aquifers ranged from 0.5 to 1.7 feet in the DNAPL and LNAPL source areas. These downward gradients were entirely reversed through the optimized extraction and injection configuration, resulting in upward head differences. A well-pronounced groundwater mound created by injection in the Gage aquifer is shown in Figures 4-7A and 4-7B. This change in vertical flow direction will tend to prevent any further downward migration in the LNAPL source areas from the MBFC into the Gage aquifer.

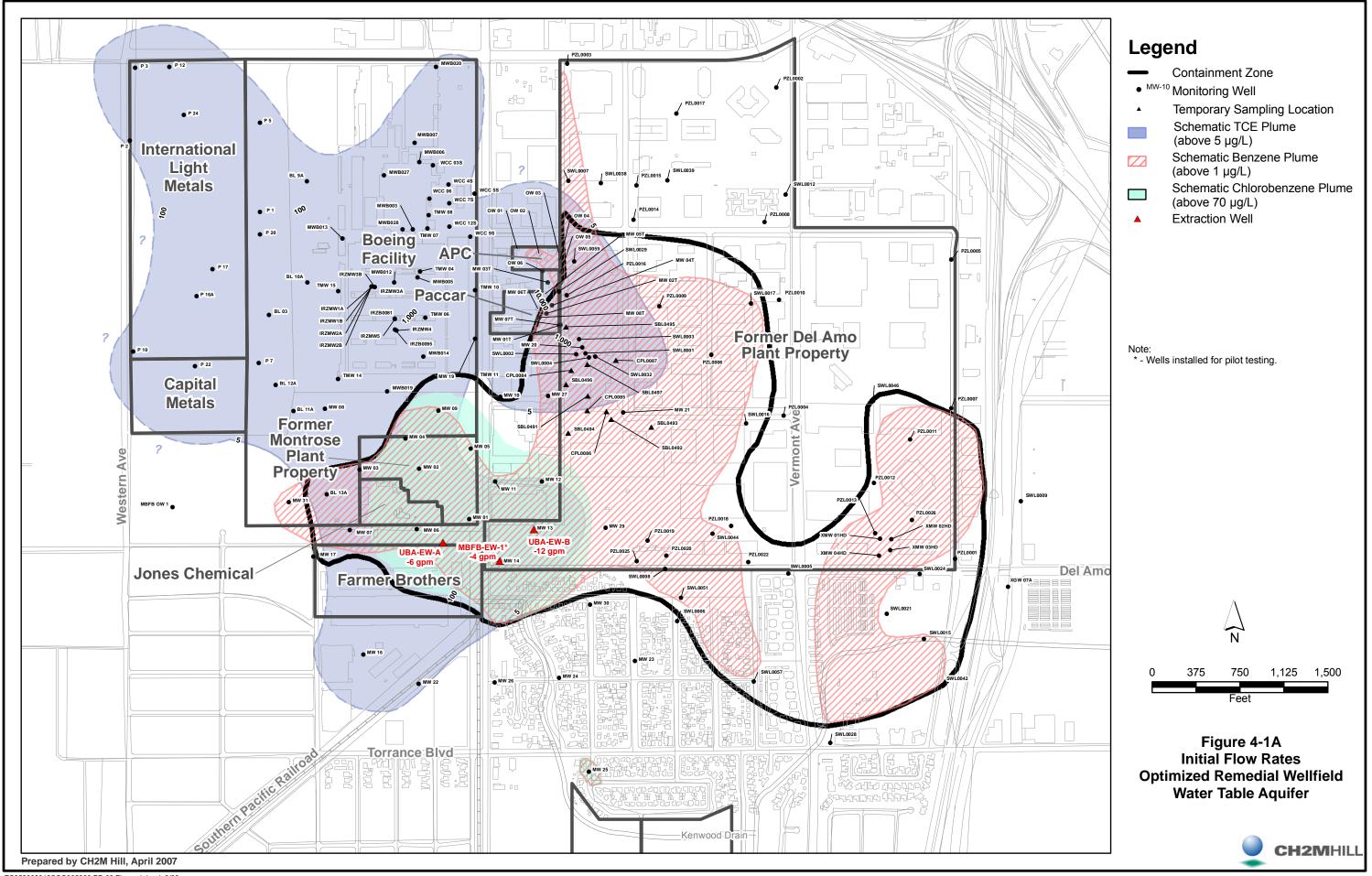
Dissolved Contamination

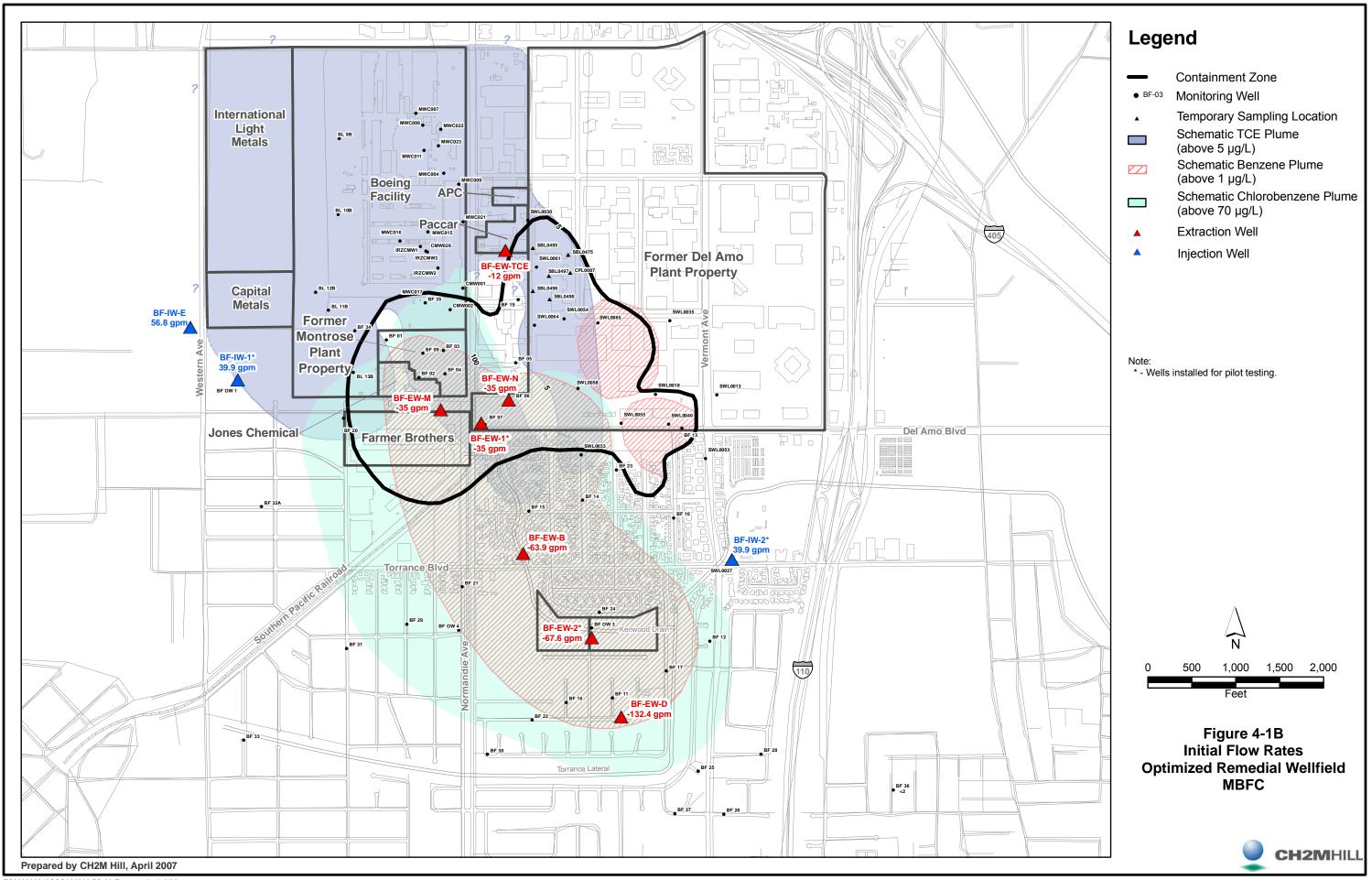
The optimized wellfield performs reasonably well at limiting adverse migration of dissolved contaminants. However, some gradient increases were observed within the dissolved contaminant distributions. In addition, activating the remedial system causes gradient directions to change in some areas, and portions of the plume reorient to match the new flow directions.

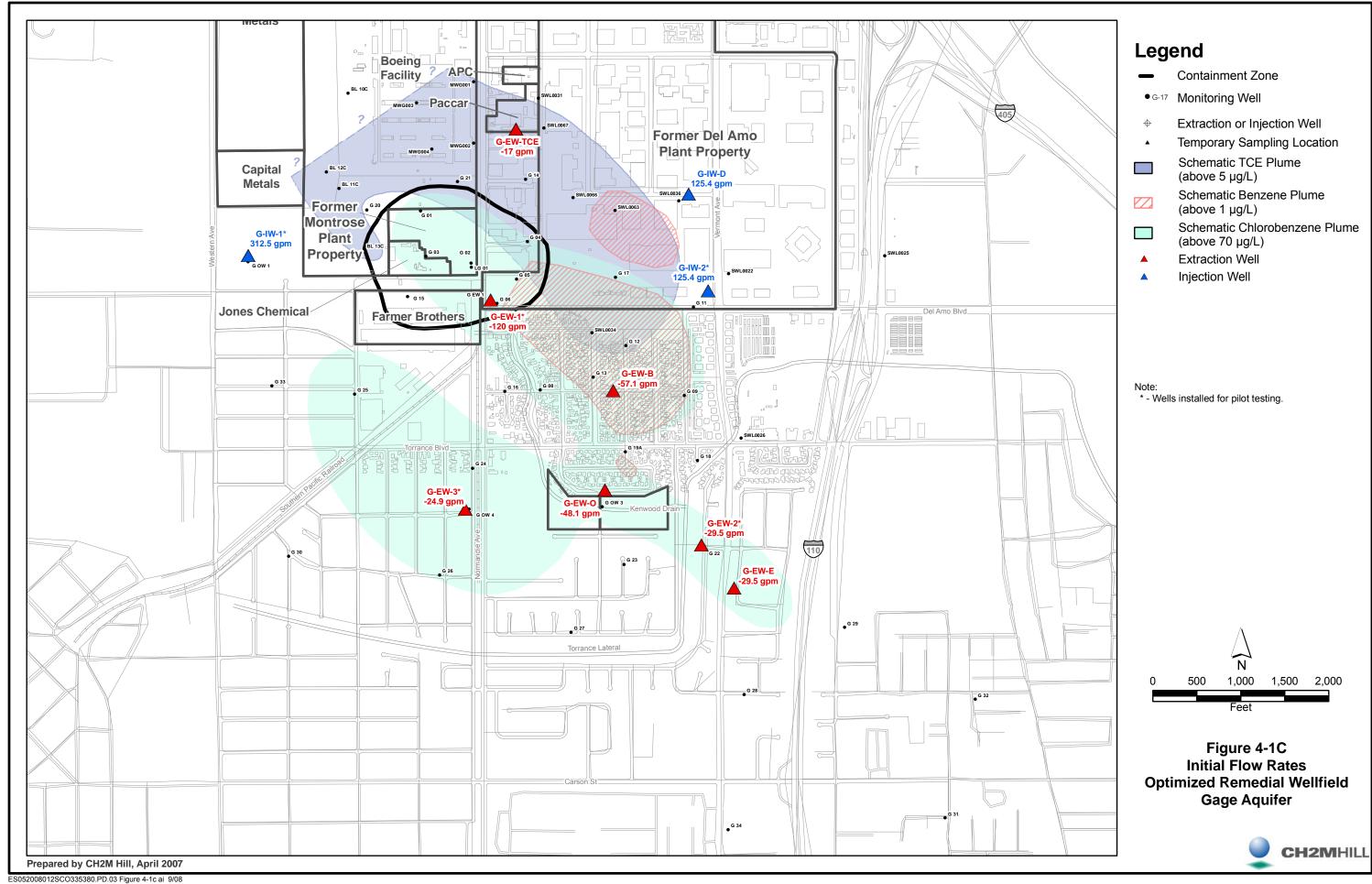
Modeling results indicate that operation of the remedial wellfield may cause some adverse migration of dissolved benzene. Figure 4-7A shows the distribution of benzene after 1 year of the remedial wellfield operations in the water table, MBFC, and Gage aquifers. This figure indicates that the benzene plume appears to be reasonably contained by natural biodegradation in the water table aquifer, where benzene occurs at the highest concentrations and has the largest extent. The modeling results indicate, however, that some slight increase in the benzene distribution may occur outside the CZ in the MBFC, near the southern boundary of the Del Amo site near the waste pits. This slight increase is attributed to the fact that the start of the remedial pumping temporarily disturbs the relative equilibrium of the benzene plume maintained by natural biodegradation and causes the plume to reorient. However, based on modeling, the reoriented benzene plume reaches a new equilibrium within a few years and does not advance from the reoriented position (Figure 4-7B).

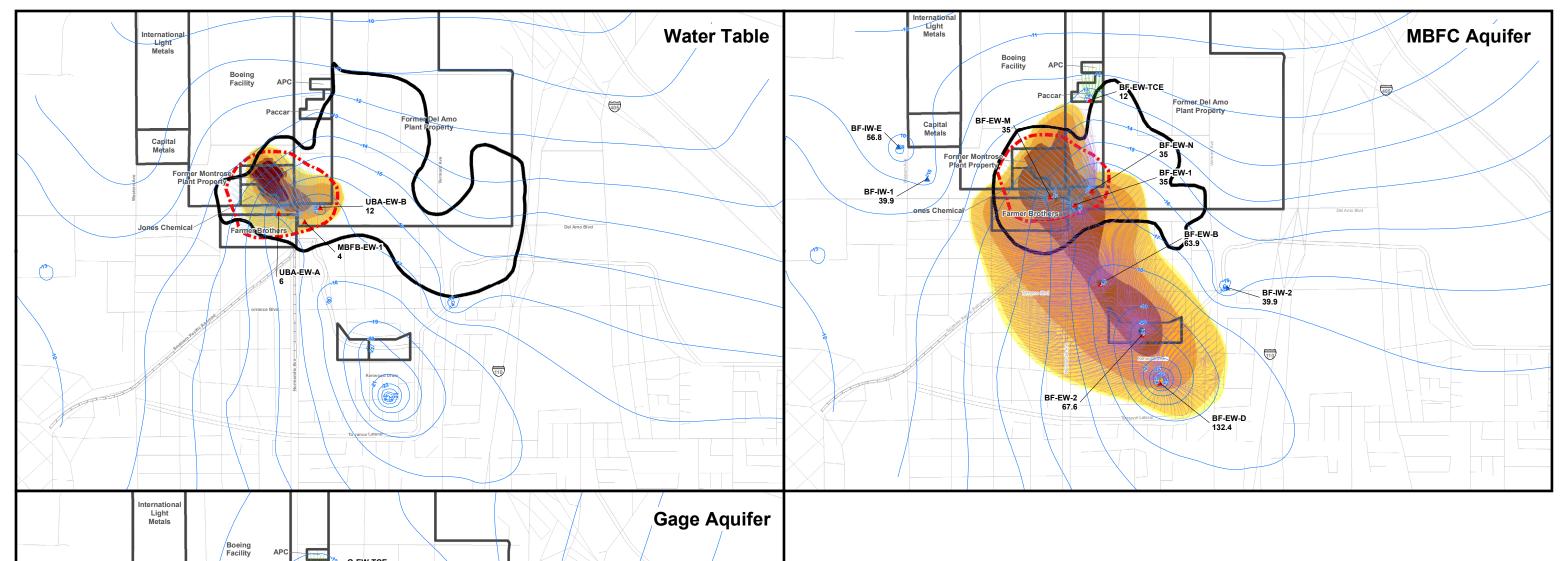
The simulated increase in the area impacted by benzene also can be attributed in part to the numerical dispersion. The impacts of numerical dispersion on the solute transport simulations of the benzene plume were demonstrated during the grid refinement analysis (CH2M HILL, 2006b). In addition, as discussed in Section 2.8.1, the concentrations of simulated benzene sources in the MBFC, near the waste pit source area, could be overestimated because the 2008 sampling data for MBFC wells located in this area were much lower than historical data used to establish the source terms in the model. Based on the above, the slight increase in the area impacted by benzene does not appear to warrant active hydraulic containment at this time. The performance monitoring program will be designed, however, to monitor benzene migration outside the CZ during the remedy implementation, and the need for active containment will be reassessed based on the results of this monitoring.

Figure 4-7A also shows that areas impacted by low-concentration benzene in the MBFC within the chlorobenzene plume, and in the Gage aquifer, also increase after 1 year of remedial pumping. However, both of these areas are contained by the remedial wells and will be remediated within the same timeframe as the chlorobenzene plume. Figure 4-7B shows that benzene in these areas is mostly remediated after 32 years of remedial operations.

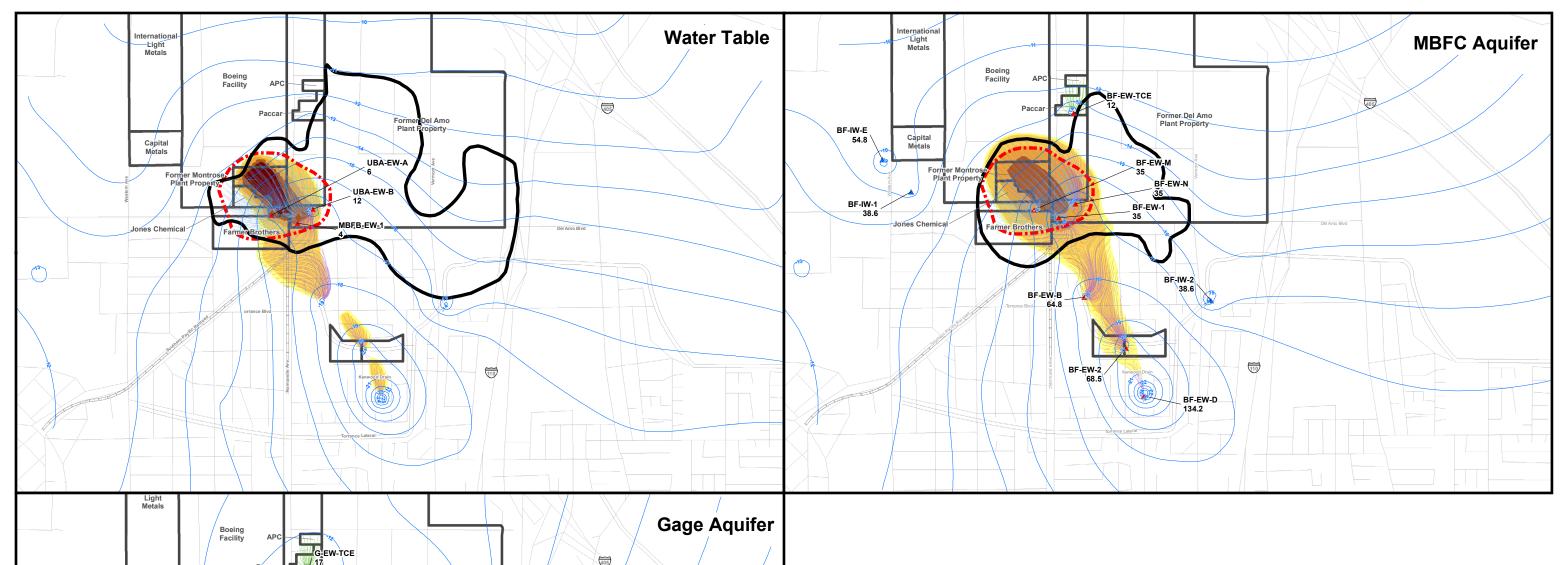




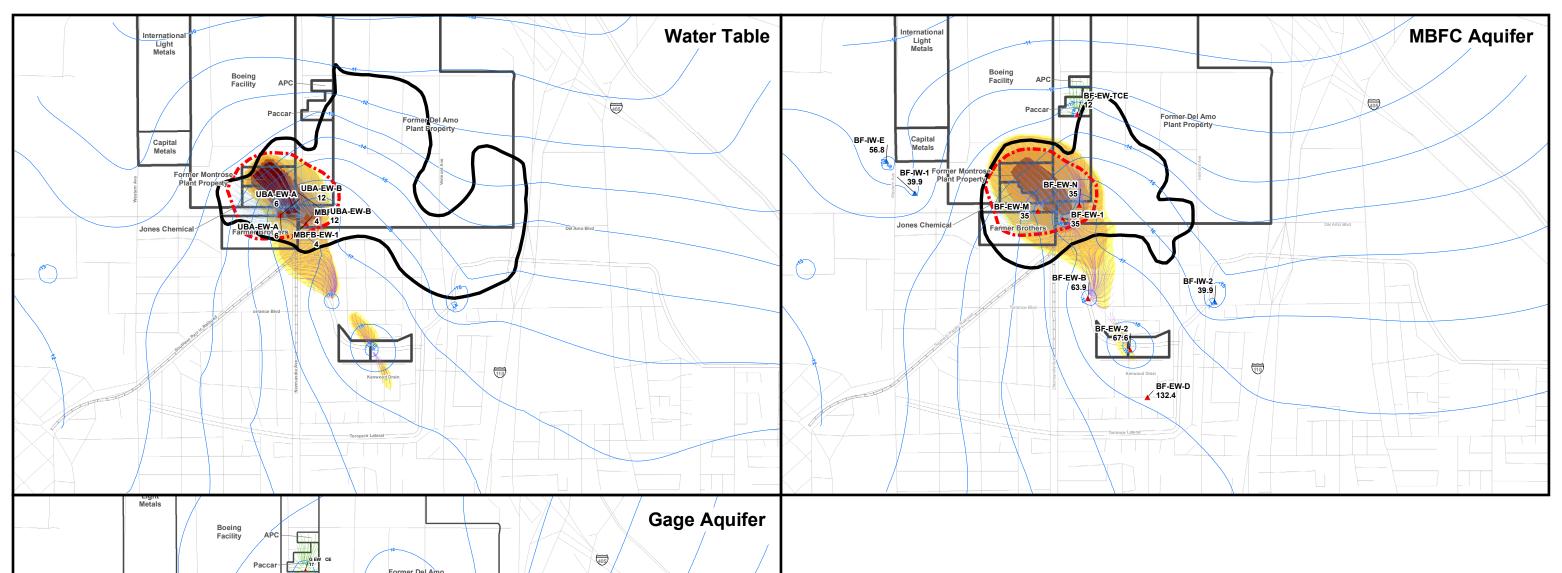


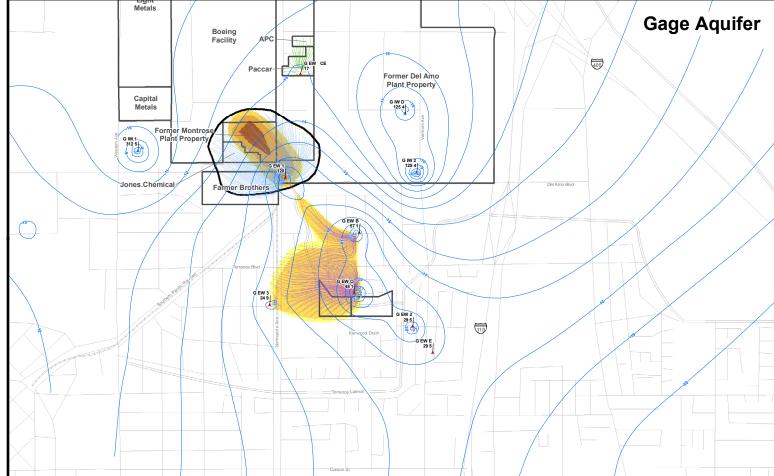


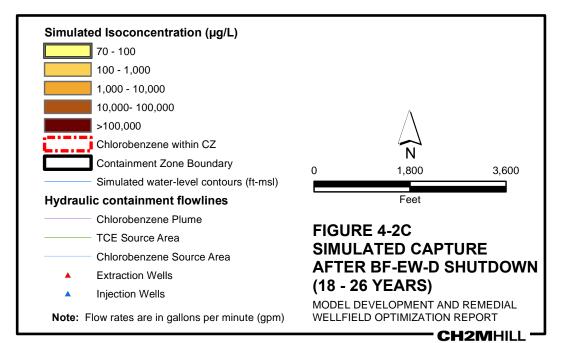


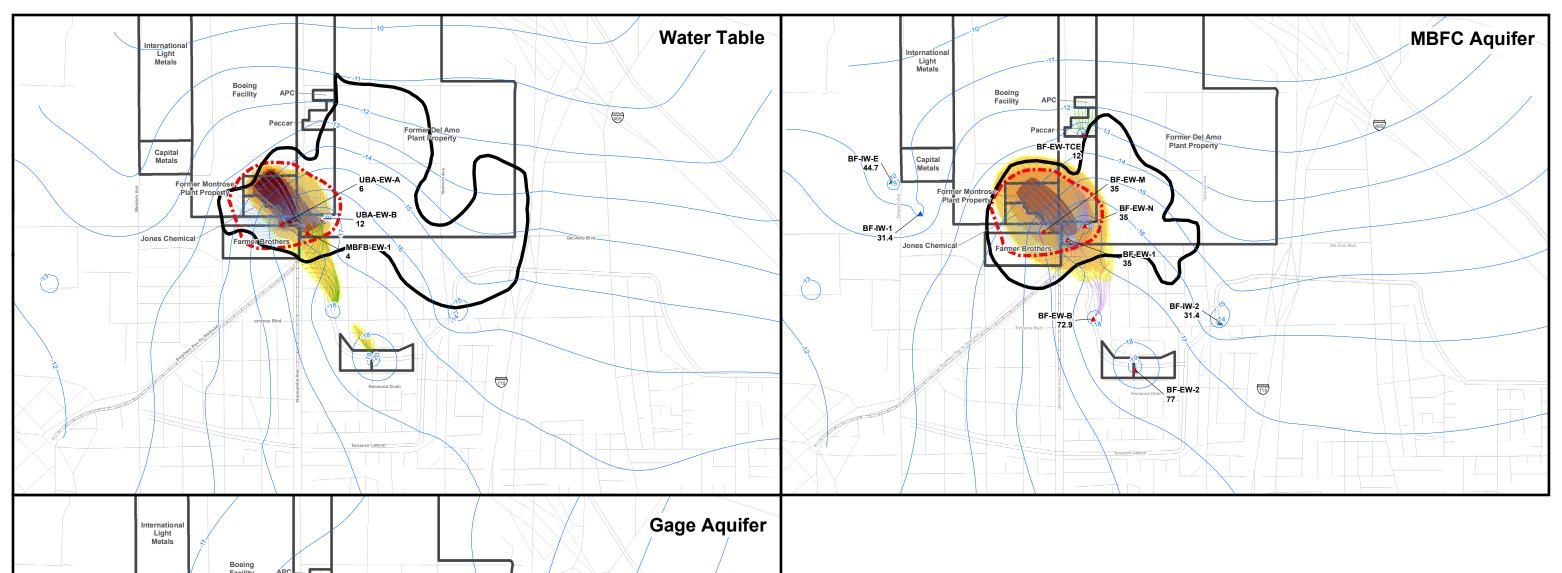


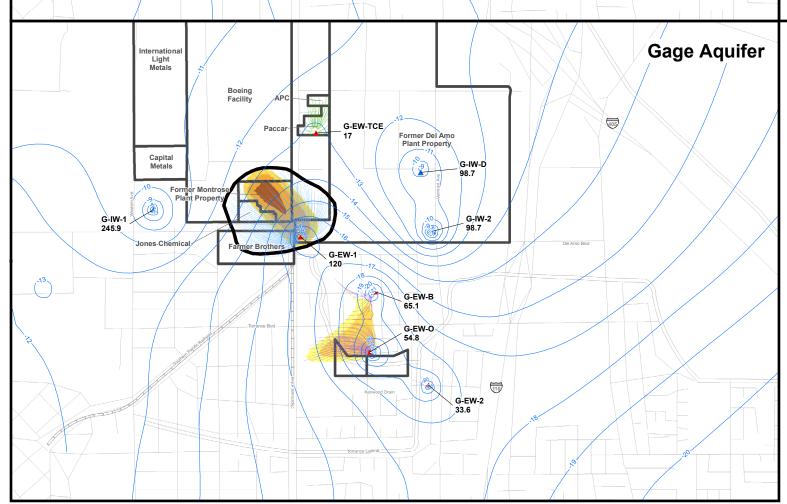


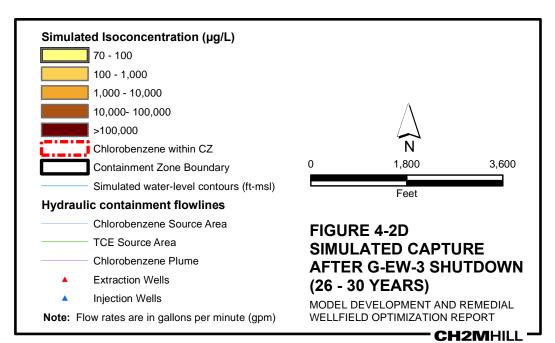


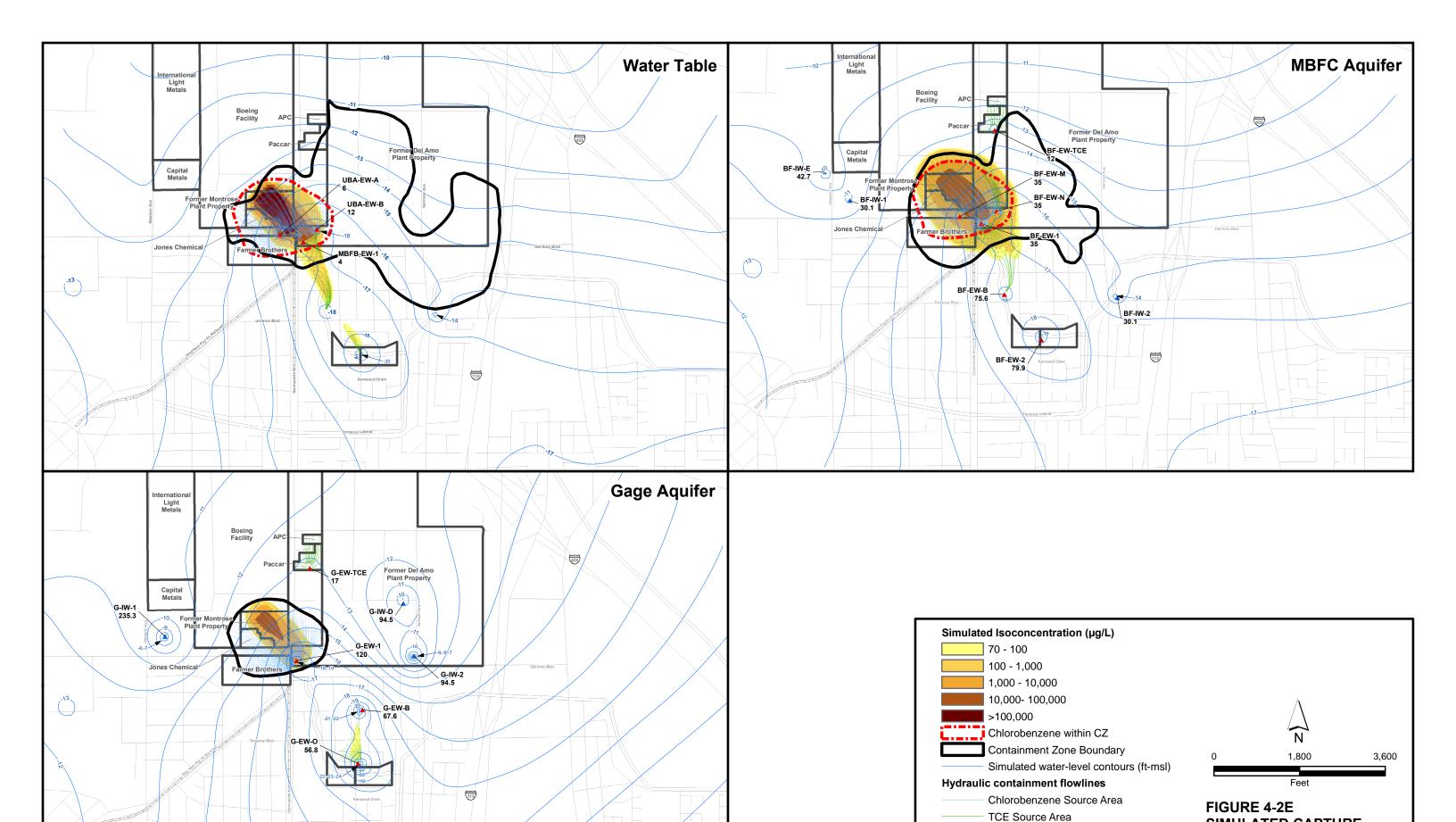












SIMULATED CAPTURE

(30 - 32 YEARS)

AFTER G-EW-2 SHUTDOWN

MODEL DEVELOPMENT AND REMEDIAL WELLFIELD OPTIMIZATION REPORT

TCE Source Area

Extraction Wells

Injection Wells

Note: Flow rates are in gallons per minute (gpm)

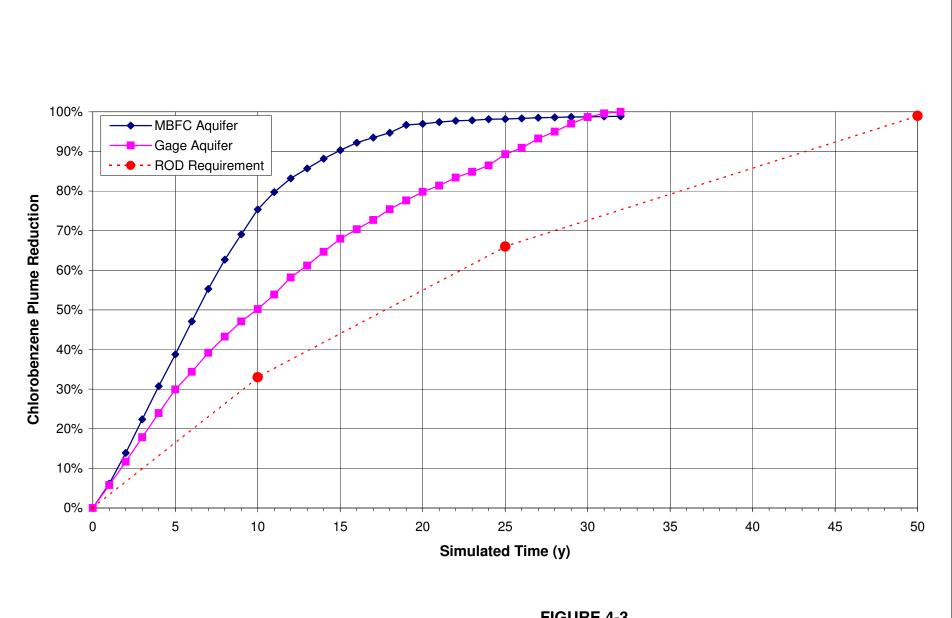
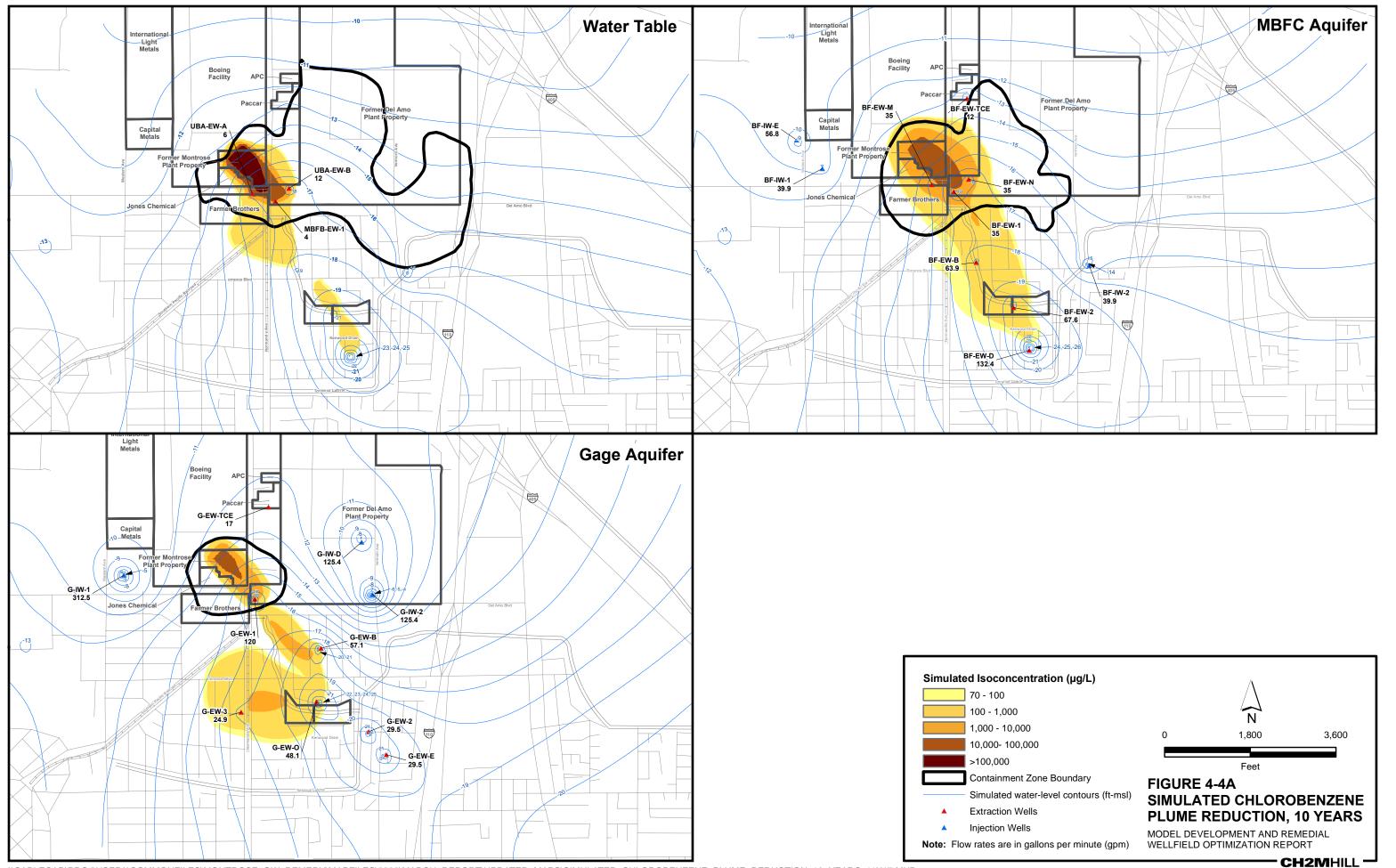
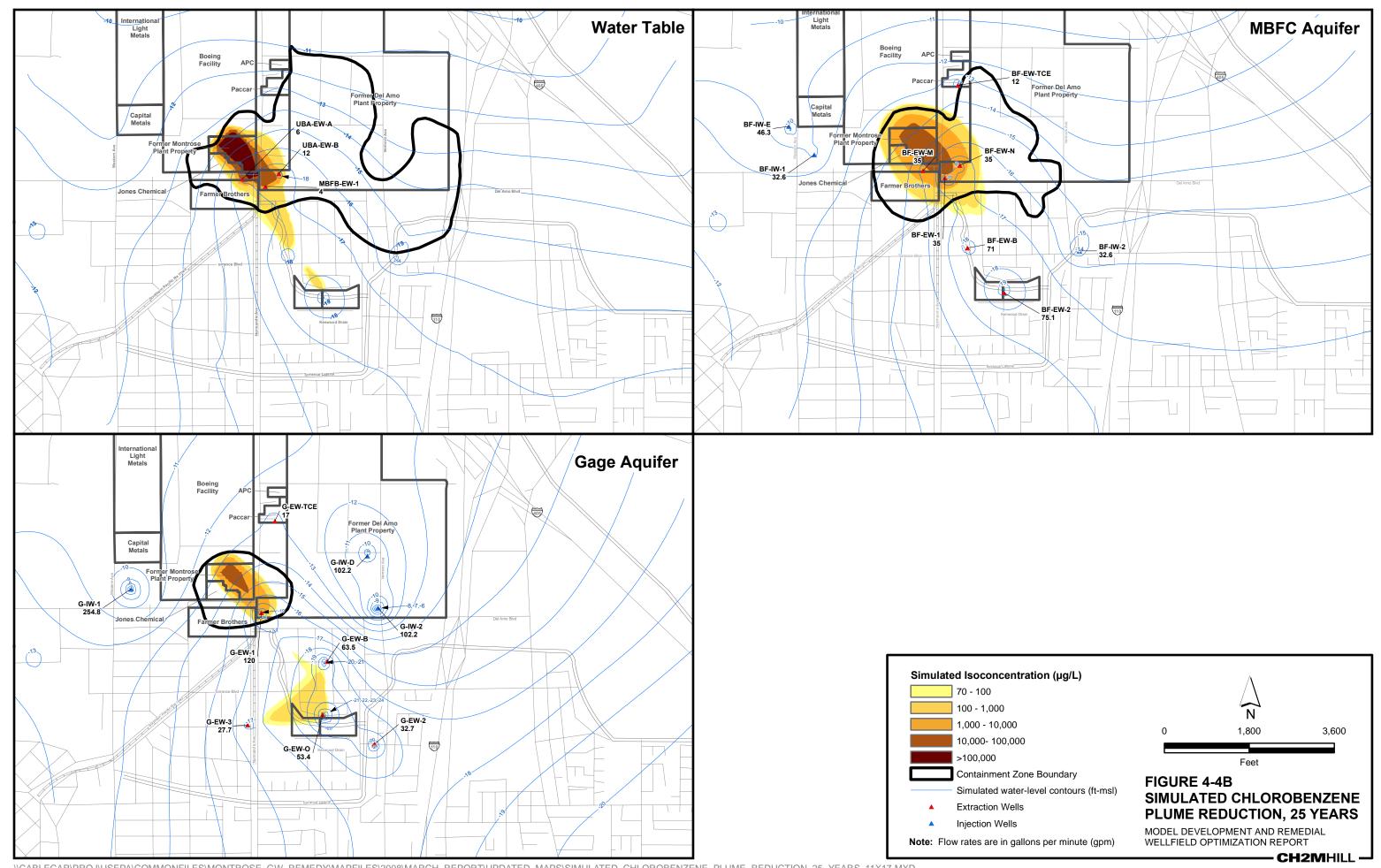
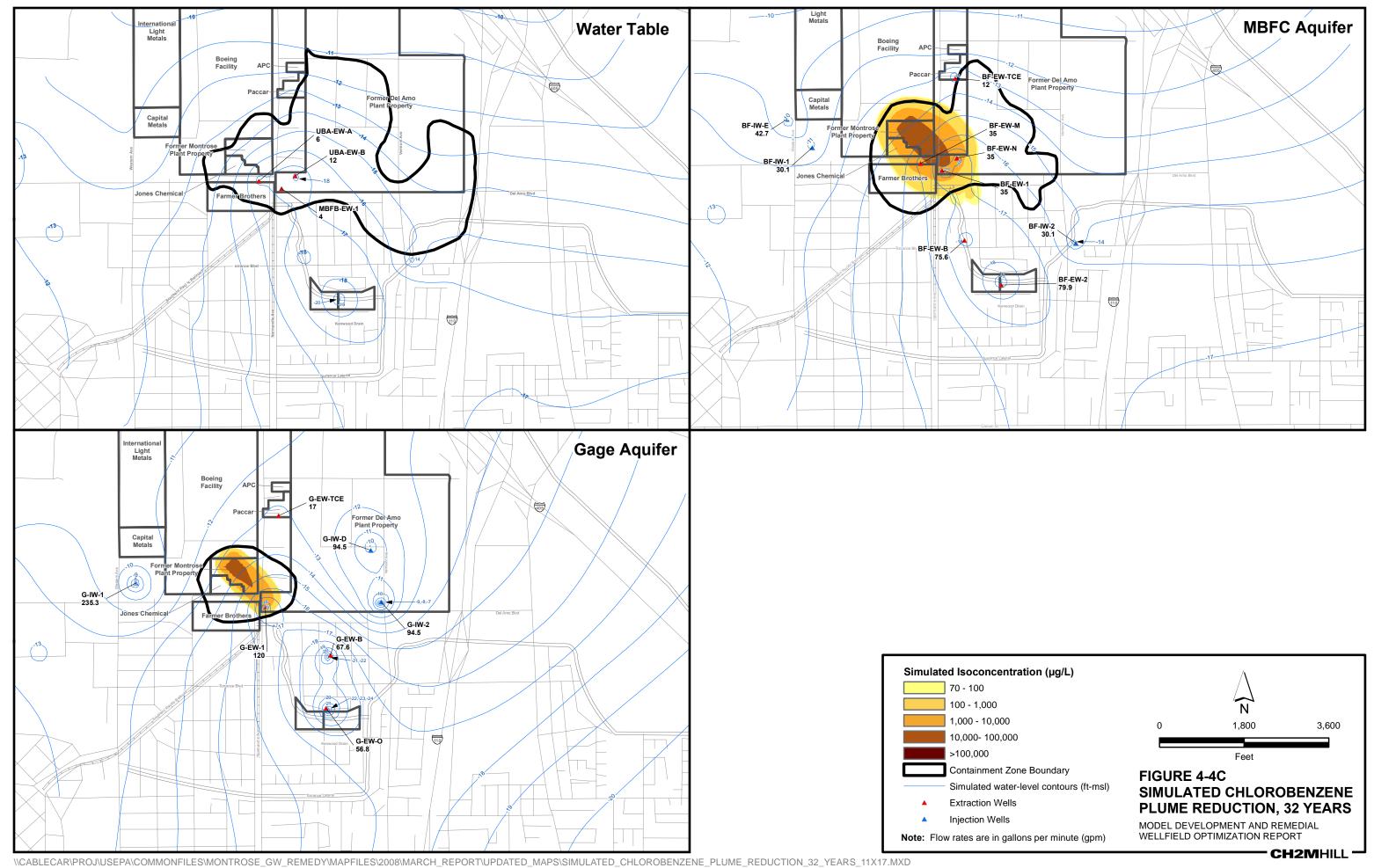


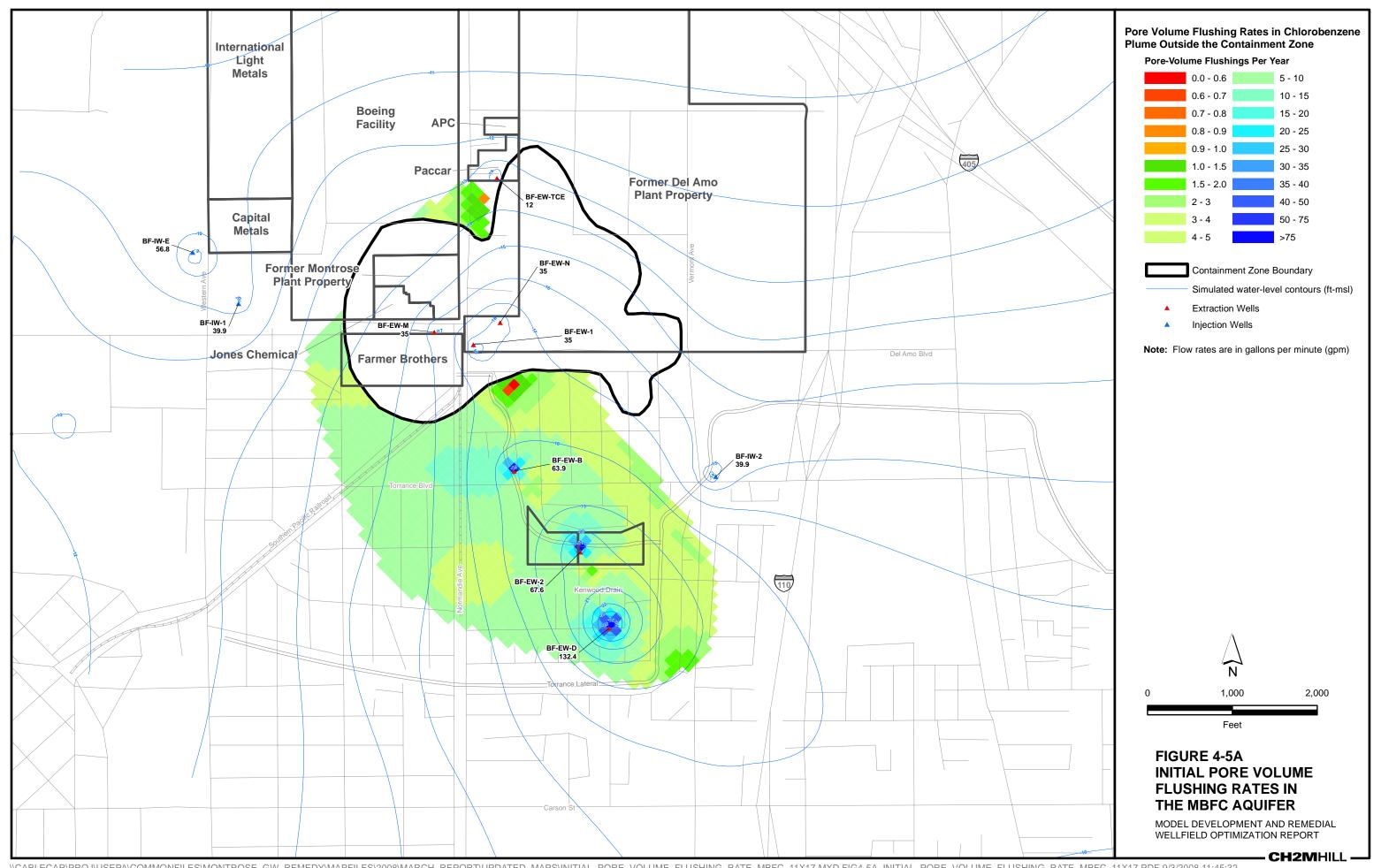
FIGURE 4-3 SIMULATED CHLOROBENZENE PLUME REDUCTION OUTSIDE THE CONTAINMENT ZONE

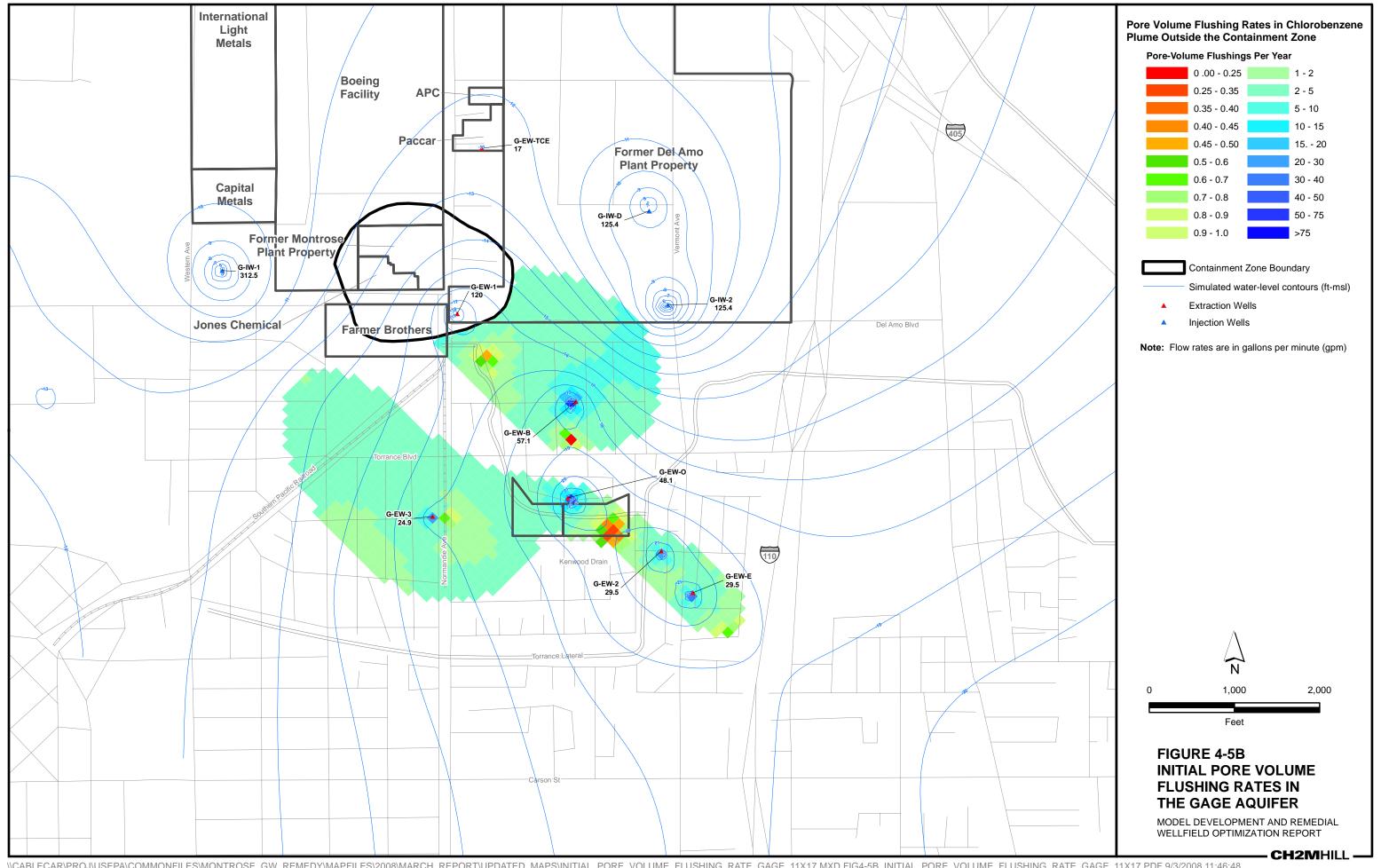
MODEL DEVELOPMENT AND REMEDIAL WELLFIELD OPTIMIZATION REPORT

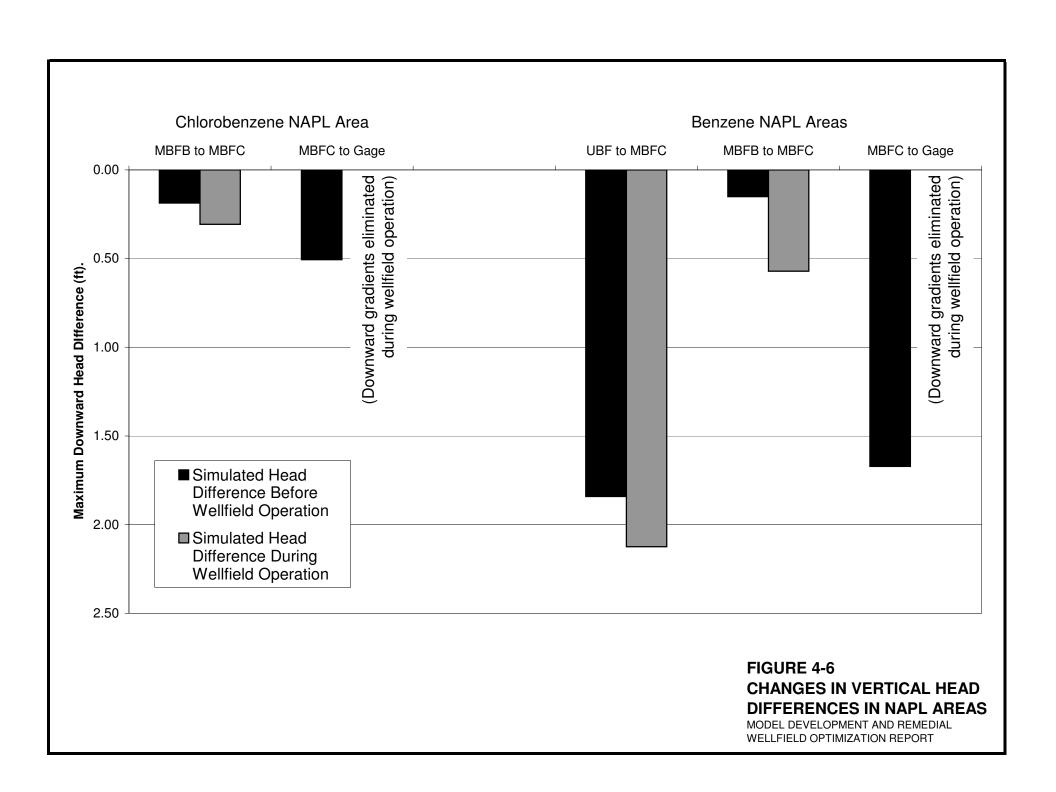


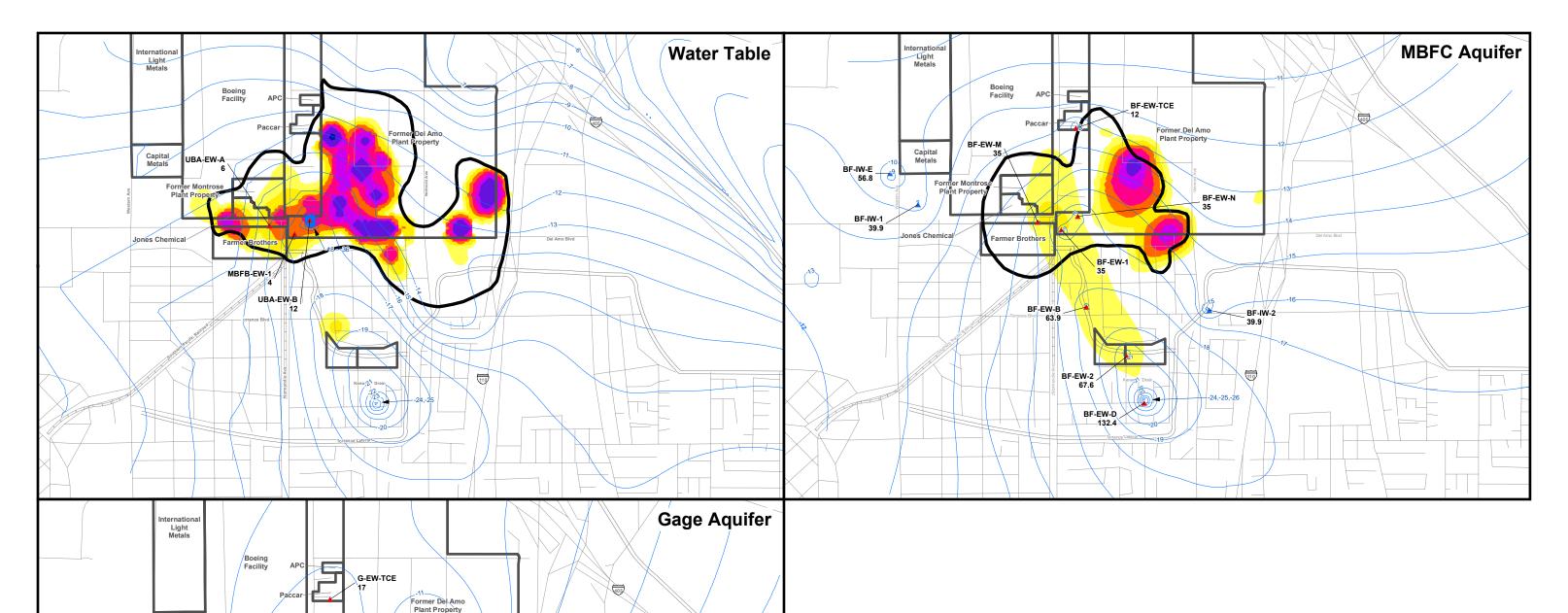




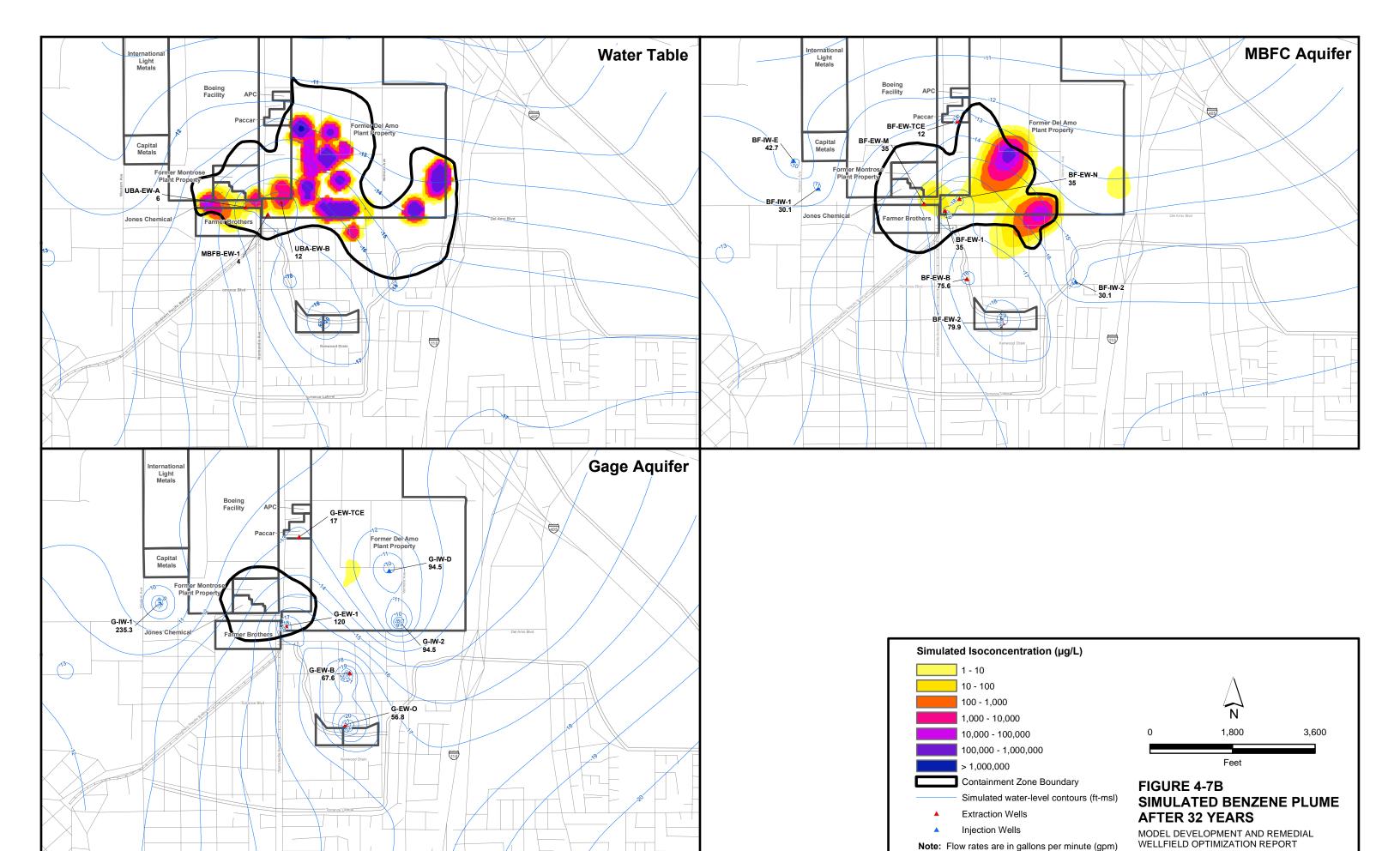












CH2MHILL

5. Wellfield Failure Analysis

This section discusses the methodology and results of failure analysis of the optimized remedial wellfield. As discussed in Section 3.1, groundwater flow and transport models are generally nonunique, and a similar quality of calibration can be achieved with a number of different model parameter combinations. Consequently, a number of models can be developed using PEST, all of which would be reasonably well-calibrated and based on equally viable hydrogeologic parameters for a given physical system. These calibrated models may differ, however, with regard to predictions pertaining to the performance of the remedial wellfield. The objective of the wellfield failure analysis discussed in this section is to account for the issues pertaining to the nonuniqueness of the model calibration, and assess if some viable calibration solutions may result in failure of the optimized remedial wellfield. The results of this analysis will be used for the development of the MACP to ensure that adequate monitoring is performed in areas of potential remedy failure. In the case of significant remedy failure under the plausible calibration scenario(s), the modifications to the optimized remedial wellfield also may be considered to ensure that the remedy is sufficiently robust to achieve ROD standards under a range of plausible conditions.

5.1 Wellfield Failure Analysis Methodology

As discussed in the Initial Calibration and Data Gap Analysis Report (CH2M HILL, 2005), there are several methods that could be used to assess the range of model predictions with regard to the performance of the remedial wellfield. One of the most comprehensive methods involves Monte Carlo analysis, in which each calibration parameter is assigned a random value, and a set of stochastic fields is generated — each based on what is known about the amount of heterogeneity prevailing within an area. While this full stochastic analysis would provide the most comprehensive information and most quantitative assessment of the modeling uncertainty, it was determined during previous modeling efforts that the MT3DMS code was not stable enough to support the use of this method for the complex RD model of the site (CH2M HILL, 2005). In addition, a stochastic approach would result in an unacceptably large increase in computational requirements. Therefore, an alternative method of predictive calibration was selected for the failure analysis to assess the predictive uncertainty of the model with regard to the performance of the remedial wellfield. The use of this method greatly reduced the cost and duration of the modeling effort.

Predictive calibration/failure analysis involves the use of "predictive targets" in the calibration process in addition to the calibration targets. The predictive targets for the failure analysis were opposites of the remediation targets used in optimization runs. For example, during wellfield optimization, a hydraulic containment target would be set so that zero particles escaping containment counted as success during adjustment of pumping rates. During failure analysis, remedial pumping rates would be held constant, and the

containment target would be set so that aquifer properties would be adjusted to permit some percentage of particles to escape containment.

In the process of the failure analysis, the model runs were performed using PEST in both calibration and predictive modes. PEST was provided with an objective function, which was the sum of squared residuals of both the calibration and predictive failure targets. This process was designed to identify (if possible) a viable combination of model parameters that calibrates the model just as well as the baseline calibration, but causes the optimized remedial wellfield to fail in achieving one or more of the ROD requirements. The objective of these simulations was to obtain the maximum range of possible plausible predictions of the calibrated model(s) with regard to the performance of the remedial wellfield (i.e., assess the predictive uncertainty of the model).

During this failure analysis, the optimized remedial wellfield was tested with regard to achieving the following remediation targets:

- Capture of the overall chlorobenzene distribution and CZ in the MBFC
- Capture of the overall chlorobenzene distribution and CZ in the Gage aquifer
- Chlorobenzene plume reduction in the MBFC
- Chlorobenzene plume reduction in the Gage aquifer
- Limiting adverse migration of benzene in the MBFC aquifer

These targets were selected because they were considered to be the most critical for the success of the remedy. If the predictive calibration runs were not able to identify a viable combination of model parameters (which would calibrate the model and cause failure of the optimized remedial wellfield to achieve the remediation targets), the optimized wellfield would be considered sufficiently robust to perform adequately under a range of plausible conditions. However, if one or more calibrated models developed during the failure analysis result in the remedial wellfield failure to meet these targets, then further modification of the remedial wellfield and/or additional performance monitoring of the potential failure areas would be required to address this issue.

5.2 Failure Analysis Results

This section presents the results of failure analysis for each of the selected remediation targets.

5.2.1 Capture of the Overall Chlorobenzene Distribution and CZ Targets

A failure analysis was performed for hydraulic capture of the chlorobenzene plume outside the CZ in the MBFC. In an attempt to verify if a failure of containment is plausible, a predictive calibration target was added to the model to cause 10 percent of the plume to escape the capture of the optimized remedial wellfield. The failure analysis runs indicated that it is impossible to identify a viable combination of model parameters that would result in both (1) a well-calibrated model, and (2) the breach of capture in the MBFC by the optimized remedial wellfield. While the size of the capture zone was slightly reduced during failure analysis compared to that under baseline calibration, the entire plume remained adequately contained (Figure 5-1A). This result demonstrated that the optimized

remedial wellfield is sufficiently robust with regard to capture of the chlorobenzene plume in the MBFC.

A similar failure analysis was performed for hydraulic containment of the chlorobenzene plume in the Gage aquifer. This failure analysis also indicated that a set of viable model parameters that can both calibrate the model and cause chlorobenzene plume capture in the Gage aquifer to fail does not exist (Figure 5-1B). Consequently, the optimized remedial wellfield is equally robust with regard to capture of the chlorobenzene plume in the Gage aquifer.

Based on the above results, the uncertainty of model predictions with regard to plume capture is relatively small. This can be explained by the fact that the accuracy of modeling predictions with regard to capture depends primarily on the quality of the flow calibration. The flow calibration of the RD model is considered to be exceptional, because it is based on a large data set of aquifer response data from multiple pilot tests covering a large portion of the modeling domain. The number of combinations of viable hydraulic properties that could calibrate the model to the pilot test results is very limited compared to other groundwater models calibrated only to static water levels, which is common practice. Consequently, the failure analysis could not identify an alternative set of hydraulic parameters that could calibrate the model to the pilot test data and cause the containment of the plume to fail. For example, the failure analysis run for the Gage plume capture was required to maintain calibration to pilot test data including data for well G-EW-2, which is located in the vicinity of the downgradient edge of the chlorobenzene plume (Figure 5-1B). However, it was determined to be essentially impossible to maintain calibration to the G-EW-2 drawdowns and substantially change hydraulic properties of the model from those identified during the baseline calibration. Because the baseline calibration parameters and remedial wellfield flow rates result in capture of a greater area than the plume in the Gage aquifer, failure analysis does not change this result.

Particle-tracking results from the wellfield optimization also were examined to identify how far the capture zone of CZ wells extended into the MBFC and Gage aquifers (Figures 5-1A and 5-1B). In both the MBFC and Gage aquifers, the simulated capture zone extended 300 to 400 feet beyond the CZ. Pilot tests were conducted at wells BF-EW-1 and G-EW-1 within the CZ. Any formal failure analysis addressing containment of the CZ would be required to maintain calibration to pilot test data from these wells. Based on PEST's inability to reduce the capture zone for the overall chlorobenzene distribution in both the MBFC and Gage aquifers, it was concluded that similar results could be expected for CZ containment. Consequently, the wellfield performance with regard to capture of the CZ was considered sufficiently robust.

5.2.2 Plume Reduction Targets

A failure analysis also was performed to assess the reliability of chlorobenzene plume reduction by the optimized remedial wellfield in both the MBFC and Gage aquifers. For the MBFC failure analysis run, a predictive failure target was added to cause plume reduction at 10 years to fail by 10 percent (i.e., for the plume to be reduced by 23 percent, instead of the 33 percent required by the ROD). This attempt to cause a failure of the plume reduction target in the MBFC was unsuccessful, although the rate of plume reduction was somewhat slower for the failure run compared to that estimated for the baseline calibration

(Figure 5-2). In the baseline calibration, the MBFC plume is reduced by 99 percent after 32 years; but in the failure analysis run, the 99 percent plume reduction was achieved after 40 years, which is still within the 50 years required by the ROD. The only scenario in which the optimized wellfield did not achieve 99 percent plume reduction in the MBFC in 50 years had unrealistic transport parameters such as a porosity of 47 percent. This value of porosity disagrees with the site conceptual model and laboratory analysis of samples at the site. Based on the above, the performance of the optimized remedial wellfield with regard to plume reduction in the MBFC is considered to be reliable and robust under the range of plausible conditions.

A similar failure analysis was performed to assess the reliability of the chlorobenzene plume reduction in the Gage aquifer (Figure 5-2). Similar to the MBFC plume reduction failure analysis, a predictive failure target was added to the model to cause plume reduction at 10 years to fail by 10 percent (i.e., for the plume to be reduced by 23 percent, instead of the 33 percent required by the ROD). This attempt to cause failure of the plume reduction target in the Gage aquifer also was unsuccessful, although the overall rate of plume reduction was somewhat slower for this failure analysis run compared to that for the baseline calibration. In the baseline calibration, the Gage plume is reduced by 100 percent after 32 years. In the failure analysis run, the cleanup time was increased to over 45 years, which is still within the 50 years required by the ROD. Other attempts to achieve failure of plume reduction targets in the Gage aquifer indicated that it is only possible by degrading the quality of the chlorobenzene calibration in the Gage aquifer to an unacceptable level. Based on the above, the performance of the optimized remedial wellfield with regard to plume reduction in the Gage aquifer is considered to be reliable and robust under the range of plausible conditions.

However, it is important to note that the uncertainty associated with the modeling simulations of the solute transport, including plume reduction times, is generally higher than that associated with the plume containment simulations. As discussed in the Initial Calibration and Data Gap Analysis Report (CH2M HILL, 2005), Kd appears to have the highest contribution to the predictive uncertainty of the model with respect to the clean up times in both the MBFC and Gage Aquifer. However, because of the significant variability of Kd in the natural systems, and because the field experiments required to quantify this parameter are complicated, costly, time-consuming, and ordinarily ineffective, uncertainty associated with Kd could not be appreciably reduced during the data acquisition efforts. In addition, the phenomenon of "slow desorption or irreversible sorption," which may have a significant impact on the actual cleanup times, could not be accounted for in the model, because of the limitations of the MT3DMS code, which does not allow for this level of complexity in representation of dissolved/sorbed contaminant interaction. As the result of this process, the actual clean up times may be longer than those estimated by the model.

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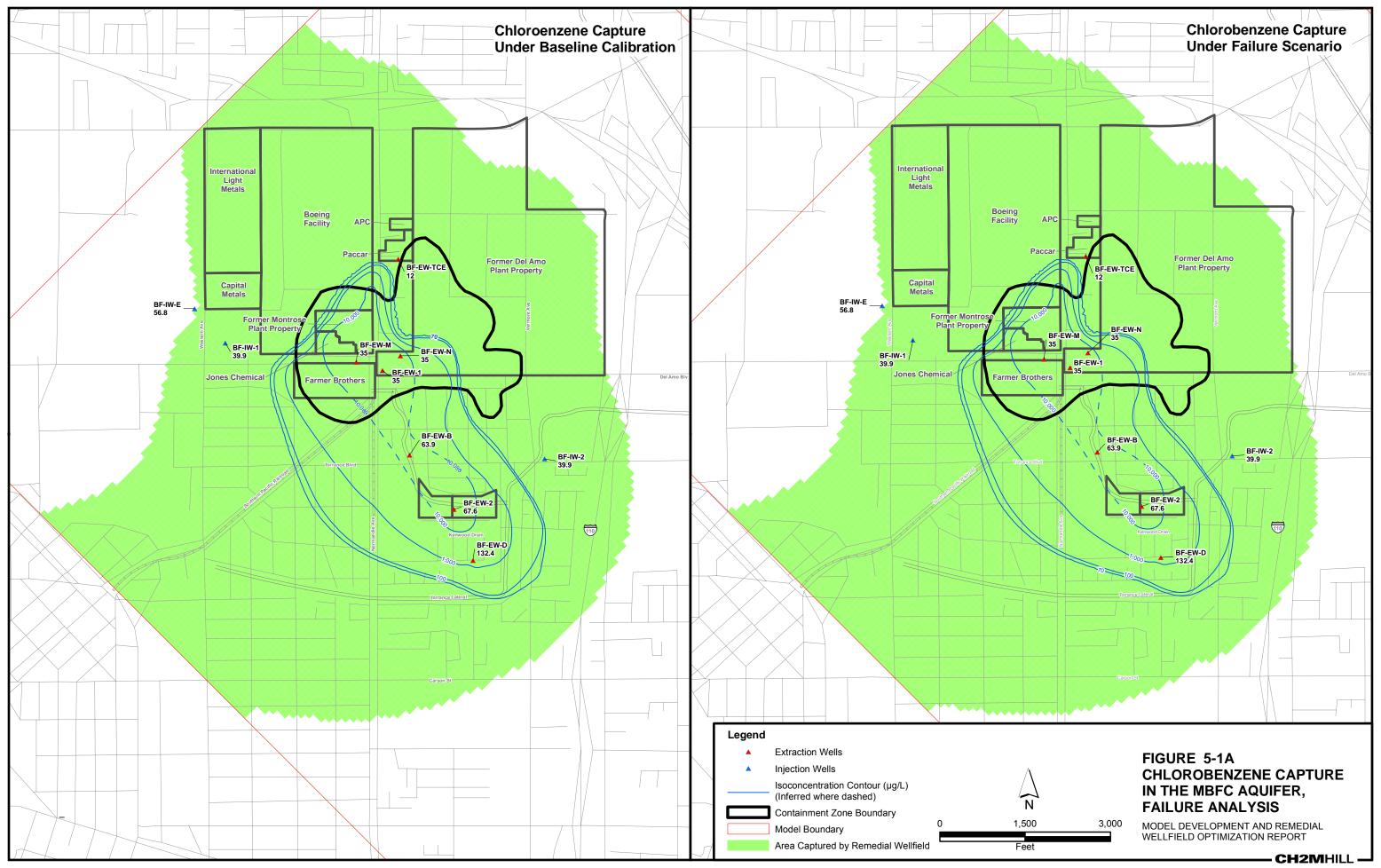
² Recent research on the ability of chemical compounds to completely desorb from a solid indicates that solid-phase contaminant concentrations can exceed the concentration predicted based on the aqueous-phase contaminant concentration and distr bution coefficient (Fu et al. 1994; Kan et al., 1997; Pignatello and Xing, 1995). This phenomenon could be explained as slow desorption or irreversible sorption. It is reported that this situation generally happens in materials that have been in contact with contaminants for long time periods and have low solid-phase contaminant concentrations, which normally are less than 20 milligrams per kilogram (Bedient et al., 1999).

5.2.3 Limiting Adverse Migration of Benzene Targets

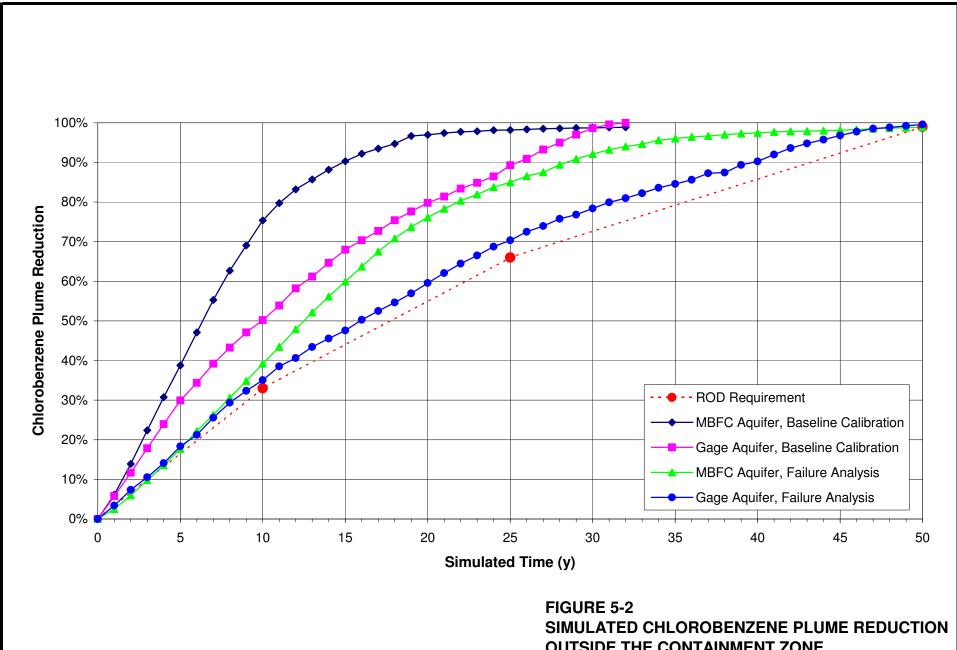
A failure analysis was performed to assess the uncertainty of modeling predictions with regard to adverse migration of benzene in the MBFC aquifer. The objective of this run was to determine whether a greater amount of adverse migration of benzene outside the CZ (compared to that simulated using the baseline calibration) could occur under a different set of viable model parameters. A predictive failure target was added to the model to induce benzene migration from the CZ. The model was then recalibrated with a different set of model parameters required to achieve this increase in benzene migration. While the failure run was able to increase the amount of adverse benzene migration in the MBFC, this increase was not significant compared to that produced using the baseline calibration (Figure 5-3).

The simulated increase in the benzene distribution was most notable near the southern boundary of the Del Amo site, downgradient of the waste pits, where benzene migrated outside the CZ. The mechanism for this adverse migration of benzene was likely similar to that observed under the baseline calibration conditions. The start of remedial pumping temporarily disturbed the relative equilibrium of the benzene plume maintained by natural biodegradation and caused the plume to reorient. However, the reoriented benzene plume reached a new equilibrium within several years and did not advance from the reoriented position.

Similar to the results produced using the baseline model, the benzene migration in the failure run is likely attributed in part to numerical dispersion. In addition, as discussed above, the modeled benzene sources in the MBFC near the waste pit source area may be somewhat overestimated based on the most recent sampling results (see Section 2.8.1). Based on these results, the slight increase in benzene migration achieved during this failure analysis does not appear to warrant additional active containment at this time. However, the performance monitoring program should be designed to address the uncertainty associated with the potential benzene migration in this area.

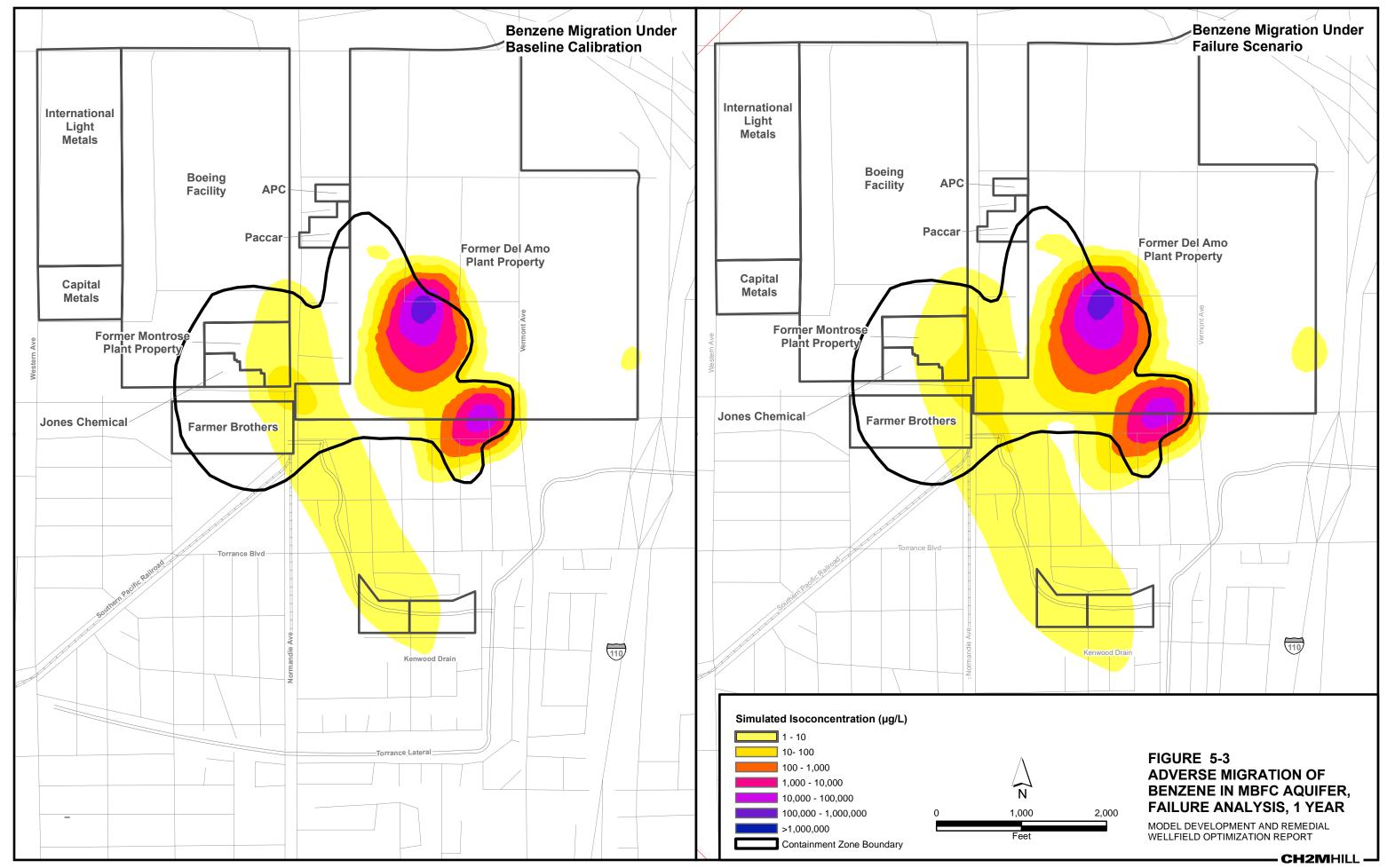






OUTSIDE THE CONTAINMENT ZONE, FAILURE ANALYSIS

MODEL DEVELOPMENT AND REMEDIAL WELLFIELD OPTIMIZATION REPORT



6. Conclusions and Recommendations

Presented below are the conclusions and recommendations developed based on the results of these modeling activities:

- 1. Numerical RD Model of the Site. The comprehensive RD model of the Dual Site was developed during these modeling activities. The model was based on the extensive body of information collected during the RI/FS and RD investigations. It was calibrated to numerous water level data, pilot test drawdown/drawup data, and solute transport data for three different contaminants including chlorobenzene, benzene, and p-CBSA. The model was reviewed and approved by EPA, Montrose, Shell, and other stakeholders as an appropriate tool for the initial optimization of the remedial wellfield and for the future evaluation of the performance of the remedial wellfield in the process of remedial actions. It is recommended, however, that the RD model be revised for the continued support of the remedial actions based on the new operational data that will be obtained after the system startup. It is expected that the initial hydraulic data obtained after the remedial system startup will be very important for the verification of the current modeling assumptions and further improvement of the RD model.
- 2. **Optimized Remedial Wellfield.** Modeling results indicated that the optimized remedial wellfield achieves and exceeds the ROD requirements and complies with the design constraints. Based on the RD model, the optimized remedial wellfield also is sufficiently robust and capable of achieving the ROD requirements under a range of plausible conditions.
 - However, please note that the specifications for the optimized remedial wellfield discussed in this report were developed based on the currently available information, and as new information is obtained—especially field operational data during remedy implementation—the wellfield may need to be reoptimized and adjusted to ensure compliance with ROD requirements. In addition, certain physical processes such as the process of slow desorption, which may have a significant impact on the actual cleanup times, could not be accounted for in the model because of the limitations of the available solute transport programs.
- 3. TCE Containment. The level of uncertainty associated with the performance of the remedial wellfield with regard to capture of the TCE plume is higher than that for chlorobenzene and benzene. This is because the TCE plume is not sufficiently characterized compared to the chlorobenzene and benzene plumes. Based on the above, additional data may need to be collected as part of the formal design and/or remedial construction of the TCE remedial system.
- 4. **Adverse Migration of Benzene.** Modeling results indicated that operation of the remedial wellfield may cause some adverse migration of dissolved benzene, which will result from reorientation of benzene distribution to the west. However, the reoriented benzene plume will likely reach a new equilibrium within a few years because of the natural biodegradation of benzene and will not likely migrate from the original

reoriented position. The modeled increase in the benzene distribution also may be attributed in part to the numerical dispersion, and in part to the potential overestimate of the strength of modeled benzene sources in the MBFC near the waste pit source area. Based on the above, active containment of benzene in the MBFC is not warranted at this time. The performance monitoring program should be designed, however, to monitor benzene migration outside the CZ during the remedy implementation, and the need for active containment should be reassessed based on the results of this monitoring.

- 5. **CZ Containment.** As required by the ROD, the CZ containment wells will operate indefinitely or until the sources of contamination are removed and the groundwater within the CZ is remediated. The flow rates of the CZ containment wells should be adjusted after the cleanup of the dissolved plumes is completed and the wells outside the CZ are shut down.
- 6. **Target Shutdown Levels.** The optimization simulations of the remedial wellfield indicated that the target shutdown level for contaminant concentrations, at which extraction wells can be turned off, should be lower than the ISGS level for chlorobenzene of $70 \,\mu\text{g}/\text{L}$. This is because the need for downgradient containment is not eliminated when the contaminant concentration in a plume-reduction well reaches the ISGS level. Based on the modeling optimization runs, using a target shutdown level of 10 to $15 \,\mu\text{g}/\text{L}$ of chlorobenzene is more appropriate than the ISGS level, because it does not result in the contaminant plume escaping downgradient containment. The target shutdown levels for the remedial wells should be further assessed during the development of the MACP.
- 7. Pumping Redistribution. The optimization simulations also indicated that (1) additional pumping should not be redistributed to the CZ containment wells (unless monitoring during remedy implementation demonstrates the lack of capture) as it may induce horizontal and/or vertical gradients in the DNAPL source area; (2) flow redistribution should be performed in a manner that does not result in creating interference (i.e., competition for capture) between the CZ containment wells and the wells located downgradient of the CZ; (3) the amount of injection into the Gage aquifer should exceed injection into the MBFC through the duration of the remedial actions because it helps to mitigate the adverse vertical migration of DNAPL and dissolved contaminants into the Gage aquifer; and (4) injection rates should be maintained at Gage injection wells (G-IW-2 and G-IW-D) located at the Del Amo site to prevent vertical migration of TCE and benzene from the CZ in the MBFC into the Gage aquifer, and these wells should be considered as the CZ containment wells.

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Electronic Copy (DVD) of Appendixes

- A Baseline Calibrated Model and Optimized Wellfield Simulation
- B Simulated Pilot Test Hydrographs
- C Simulated Chlorobenzene, Benzene, and p-CBSA Chemographs
- D Modifications to MT3DMS Code
- E 3D Animations of Optimized Wellfield Performance









